

Aspects of Quantum Coherence

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This dissertation is the result of work carried out in the Theory of Condensed Matter Group of the Cavendish Laboratory, Cambridge, between October 2000 and June 2005. Except where explicit reference is made to the work of others, the work contained in this dissertation is my own, and is not the outcome of work done in collaboration. No part of this dissertation has been submitted for a degree, diploma or other qualification at this or any other university. The total length of this dissertation does not exceed sixty thousand words.

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Preface

In this work our aim is to study several aspects related to quantum coherence as understood to correspond with the non-classical behaviour that can be observed for certain particular states of a physical system. In particular we are interested in the possible mechanisms that result in dynamically induced transitions between quantum and classical regimes. The thesis is organized as follows:

The first chapter dubs as an introduction and serves to set out the basic philosophy underlying the questions addressed in this thesis. It also presents some elementary properties of states and state spaces in Quantum Theory including what we have chosen to define as classical and quantum behaviour.

In chapter 2 we study some of the aspects related to observing quantum behaviour and of the properties of our main definition of classicality (and quantumness). Here we also study some of the restrictions imposed on measurements by the existence of globally conserved quantities (Wigner-Araki-Yanase theorem) and their relationship to weak measurements coupled to postselection.

In the following chapter we review some of the basic tools used in the description of open quantum system dynamics that will be applied in other chapters.

In chapter 4 we review the basics of decoherence and analyse the importance of the choice of initial conditions when trying to study the dynamical emergence of classical behaviour within Quantum Theory.

Next we study the other direction of the transition and focus on how to obtain pure quantum states from states that originally were classically mixed.

Along the same lines, in chapter 6 we cover some topics related to the production of pure quantum states from measurements. We pay special attention to a model of the non-selective continuous monitoring of a system coupled to another unmonitored system.

Lastly we explore some of the possible similarities between the theory of phase transitions and the quantum-classical transition.

We must emphasize that all the work done in this thesis assumes that Quantum Theory is generally valid (at least within a broad enough range of energies). Thus, when we say that a state is “classical” we will mainly be referring to one of all the possible states contained in Quantum Theory, but that is susceptible to being interpreted as corresponding to “classical” behaviour. Similarly when we speak of creating a “quantum”, or “quantum coherent”, state we mean that the system has evolved to this state from one of the “classical” ones, but all of these still correspond to valid states within Quantum Theory.

In the opinion of the author the main original contributions that can be found in this thesis are the following:

- The recognition of the relationship between the Wigner-Araki-Yanase theorem and weak measurements coupled to postselection (sections 2.2 and 2.4);
- A mathematical proof of the possible ambiguities arising when two observers try to decide if a state corresponds to quantum or classical behaviour (section 2.6);
- The implications of initial correlations in decoherence models. In particular how the choice of certain (correlated) initial conditions can result in residual coherence and the production of pure quantum states in a model that otherwise results in ideal decoherence when (locally equivalent) uncorrelated initial conditions are used (section 4.2);
- Various results related to the production of quantum states from initially classical states (sections 5.2 to 5.4);
- The analysis of the inverse of a generalized depolarizing channel (section 5.7);
- The study of a model of the non-selective continuous monitoring, in the quantum Zeno limit, of a subsystem A interacting with an unmonitored subsystem B . In particular the absence of the purification of B , which has been previously predicted in the selective case, but the possibility of coherent dynamics for B (section 6.4);
- The identification of the loose equivalent of a broken symmetry and order parameter in the quantum-classical transition (section 7.2).

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To Elsa and my mother...

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Chapter 1

Definitions and Clarifications of Quantum Coherence

1.1 Some interpretational issues

Throughout the thesis we will be making constant reference to concepts such as *classical* and *quantum behaviour*. Even though we accept the general validity of the mathematical machinery of Quantum Theory this is open to certain interpretational difficulties. For example, if we were to follow a many-worlds type of interpretation [Everett 1957], one could argue that such a distinction is irrelevant. However, in this thesis we will mainly adhere to what can be primarily called the Copenhagen interpretation, in which it does make sense to make a distinction between classical and quantum behaviour (for a collection of what are the main concepts usually associated with this interpretation see [Stapp 1972] and [Bub 1997]).

Notwithstanding, if we accept the existence of two distinct types of behaviour, we soon run into difficulties. Broadly, we have that Quantum Theory is the result of attempts to account correctly for an extremely wide range of experimental results that, up to the beginning of the 20th century, could not be explained by existing “classical” theories (for a historical introduction and a collection of the main original papers -translated into English- see [van der Waerden 1967]). However, as is usually the case with any novel theory, these new tools carried with them certain interpretational issues. So-called quantum effects are considered to be real, they are observed in the laboratory, but their explanation does not coincide with our classical prejudices (which mainly coincide with what we observe in everyday life outside the laboratory). In other words, we basically have that, for certain experiments,

$$\langle A \rangle_{\text{quantum}} = \langle A \rangle_{\text{experiment}} \pm \Delta,$$

where $\langle A \rangle_{\text{quantum}}$ is the expected value of the property A as predicted by Quantum Theory, and $\langle A \rangle_{\text{experiment}}$ is the mean value of the property obtained in the laboratory experiment, with an associated uncertainty Δ . Then, when it is said that Quantum Theory is non-classical, it is generally implied that

$$\langle A \rangle_{\text{quantum}} \neq \langle A \rangle_{\text{classical}},$$

where $\langle A \rangle_{\text{classical}}$ is the value predicted by the so-called classical theory. The problem is that the “definition” of what $\langle A \rangle_{\text{classical}}$ is depends on what one chooses to term as classical. In other words, it depends on what the particular observer is used to calling classical behaviour.

Nevertheless, there are experimental examples that seem to be extremely paradoxical from any perspective based on our usual macroscopic everyday experiences. An illustration of how awkward things can get is the situation of Schrödinger's cat in his famous thought experiment [Schrödinger 1935], whose main concepts have been experimentally verified for macroscopic objects [Friedman *et al.* 2000] (for a general review of interference in macroscopic samples we refer the reader to [Das Sarma *et al.* 1995]).

Thus, it seems only natural to ask how do our everyday experiences, our classical prejudices, fit within such a successful theory as Quantum Mechanics when applied to the numerical predictions of so many experiments (or alternatively, how is Quantum Theory capable of emerging in a world consistent with our classical intuition). This is the origin behind the myriad of interpretations for Quantum Theory¹, and of most of the alternative theories attempting to replace (or complement) Quantum Mechanics (e.g. [’t Hooft 2001] [Adler 2004]). It is also, one of the main philosophical precepts being *implicitly* used in this thesis; we have chosen to accept Quantum Theory as valid and then attempt to understand the appearance of classical and non-classical behaviour within it.

However, we have that any definition of classicality (and of quantumness) will almost certainly be context dependent, and we could probably carry on *ad infinitum* trying to define what should be considered as classical, and what as quantum, within each of the possible interpretations. This is not the main objective of the present thesis. Instead we will take a more pragmatic approach. In practice, the definitions we will use for classical and quantum behaviour will have the versatility of being relevant for this type of philosophical discussion within the context of decoherence theory [Zurek 2003] and the Copenhagen interpretation, but they will also be of practical relevance since what we will often call quantum behaviour coincides with some of the necessary states of matter for applications such as quantum computing [Nielsen & Chuang 2000].

1.2 Set theoretic interlude

Following our previous discussion, let us try to give a more mathematical formulation of certain aspects of the problems we would like to study in this thesis.

Let us denote the state of the system under study by ρ and the collection of all possible states by S . Ideally, one of the questions we would like to address is: Can we define some sort of criterion that will allow us to state whether a given state ρ corresponds to *classical* (C) or to *quantum* (Q) behaviour?

More specifically, does it make sense to define the sets² $\tilde{C} \subseteq S$ and $\tilde{Q} \subseteq S$ such that

$$\tilde{C} = \{\rho \in S \mid \rho \text{ is a classical state}\}, \quad (1.1)$$

and

$$\tilde{Q} = \{\rho \in S \mid \rho \text{ is a quantum state}\}. \quad (1.2)$$

If so, what are the conditions that ρ must satisfy to belong to one or the other set? Obviously this will depend on our choice of definition of what is to be considered as quantum or classical behaviour.

¹For an introduction to some of the main concepts underlying each of the most “accepted” interpretations see [Bub 1997] and [Schlosshauer 2004].

²Throughout this thesis we will denote sets by a tilde.

Furthermore, given a certain criterion for the definition for these sets, what is the relationship between them? Intuitively one would expect the two types of regimes to be clearly distinct and hence

$$\tilde{C} \cap \tilde{Q} = \emptyset. \quad (1.3)$$

Although this empty intersection is debatable, it is our opinion that most of the existing experimental evidence (at least as it is interpreted in most of the generally accepted theories) suggests that these two regimes, the classical and the quantum, exhaust all the possibilities. Therefore we will take for granted that

$$\tilde{C} \cup \tilde{Q} = S \quad (1.4)$$

It must be mentioned that there exist alternative theories that consider the possibility of other regimes different from what we would normally call classical or quantum. For example Valentini proposes a theory where “ordinary” quantum mechanics corresponds to the equilibrium regime of some sort of generalized hidden variable theory [Valentini 2003]. However, in this thesis we will not consider this type of possibility. In fact, our general philosophy will be that it is sufficient to define what we will mean by classical behaviour, and we will term all other phenomena corresponding to non-classical behaviour as quantum. Thus, we will accept that, once we have defined the set of classical states \tilde{C} , the quantum set \tilde{Q} will be given by:

$$\tilde{Q} = \left\{ \rho \in S \mid \rho \notin \tilde{C} \right\}. \quad (1.5)$$

We are aware that such a crisp division between quantum and classical behaviour is somewhat artificial and does not coincide exactly with the general view that the frontier between \tilde{C} and \tilde{Q} is fuzzy, as is typically exemplified by the wave-particle duality³. In fact, some aspects of the ambiguity of such a partition will be highlighted in section 2.6. Nevertheless, a clear cut division such as the one implied in (1.5) will provide us with a suitable criterion on which to base our discussions of the problem of the transition from Q to C, and from C to Q. As well, since such a partition is implicitly used in most decoherence studies [Zurek 1993] [Giulini *et al.* 1996] it will allow us to compare our results with those in the existing literature. Thus, we will use this general scheme to define quantumness and classicality in section 1.5.1, and this will be the main approach used throughout this thesis.

Subject to the previous caveats, the main objective of this thesis is not so much to define quantum and classical behaviour but instead, given a certain dichotomic splitting of the state space, how can one go from one type of behaviour to the other, and back again. In fact, although our splitting of the state space might not be ideally suited for a philosophical discussion of what is quantum or classical behaviour, the partitions we will use will indeed correspond to cases of practical interest (e.g. for applications in quantum computers).

Thus, given a partition of S , we will consider how the states in each partition are affected by the action of generalized maps $\hat{\Lambda}$ ⁴ (such as those described in chapter 3). We will accept that these maps can represent almost any kind of process, e.g. it could be the dynamic evolution of an

³One of the most recent (and beautiful) examples of this is the experimental verification of the Kapitza-Dirac effect where a standing light wave is used as a grid to observe the interference of free electrons [Freimund *et al.* 2001].

⁴In the case where the state is represented by an operator, the map $\hat{\Lambda}$ is generally called a *superoperator*. This type of object will be denoted by a circumflex accent. (The only exception where the circumflex accent will be used to denote an object different from a superoperator will be in chapter 7 where it will also be used to denote field operators).

open or closed system, or it could be a series of projectors associated with an ideal measurement, or even a composition of the previous. The only condition we will require of them is that they map a subset of states, $\tilde{D} \subseteq S$, into other states in S , viz:

$$\hat{\Lambda} : (\tilde{D} \subseteq S) \rightarrow (\hat{\Lambda}(\tilde{D}) \subseteq S).$$

To ease the description of the problem of transitions between partitions let us introduce the following notation:

By $\text{dom} \{ \hat{\Lambda} \} \subseteq S$ we will read the domain of definition of the transformation $\hat{\Lambda}$ (although the proper domain of definition, as is usually understood in a mathematical context, may include objects outside of S , we will only be interested here on the action of $\hat{\Lambda}$ on states, and therefore we will limit the meaning of the term domain of definition to those elements that belong to the state space S).

Also, by $\text{range} \{ \hat{\Lambda}|_{\tilde{A}} \}$ we will understand the range of the map $\hat{\Lambda}$ when its action is restricted to the set $\tilde{A} \subset \text{dom} \{ \hat{\Lambda} \} \subseteq S$ (or in other words the image of \tilde{A} under the action of $\hat{\Lambda}$).

Using this notation one possible formulation of the question of *decoherence*, the transition from quantum to classical behaviour ($Q \rightarrow C$ transition), could be stated as: Given an initial state $\rho_0 \in \tilde{Q}$ what are the maps $\hat{\Lambda}$, if any, such that $\hat{\Lambda}[\rho_0] \in \tilde{C}$ whenever $\rho_0 \in \text{dom} \{ \hat{\Lambda} \}$?

An alternative formulation of decoherence could be to fix the map $\hat{\Lambda}$. In this case we would like to determine if a set $\widetilde{Dec} \subseteq \tilde{Q}$, and $\widetilde{Dec} \subseteq \text{dom} \{ \hat{\Lambda} \}$, exists, and if so which are its elements, such that for the given $\hat{\Lambda}$ it satisfies

$$\text{range} \{ \hat{\Lambda}|_{\widetilde{Dec} \subseteq \tilde{Q}} \} \subseteq \tilde{C}. \quad (1.6)$$

The question of decoherence has been extensively studied in the literature, however a question that has been somewhat overlooked, and that could have important implications, is the study of the transition from the classical to the quantum regime ($C \rightarrow Q$ transition). That is, given an initial $\rho_0 \in \tilde{C}$ what are the maps, if any, such that $\hat{\Lambda}[\rho_0] \in \tilde{Q}$ whenever $\rho_0 \in \text{dom} \{ \hat{\Lambda} \}$.

As in the previous example, an alternative formulation of this quantum *coherence creating process* (CCP) could be to fix the map $\hat{\Lambda}$, and determine if a set $\widetilde{CCP} \subseteq \tilde{C}$ ($\widetilde{CCP} \subseteq \text{dom} \{ \hat{\Lambda} \}$) exists, and if so which are its elements, such that for the given $\hat{\Lambda}$ we have

$$\text{range} \{ \hat{\Lambda}|_{\widetilde{CCP} \subseteq \tilde{C}} \} \subseteq \tilde{Q}. \quad (1.7)$$

All these concepts will be implicitly used in the rest of the thesis.

1.3 States, density matrices, and pure states

There are several ways to formulate Quantum Theory. For example, compare the different mathematical approaches in [Bohm 1951], [Thirring 1981 vol. 3], [Sakurai 1994], and [Sewell 2002]. However, one of the most common ways is to consider that the observables, or measurable quantities of the system, correspond to operators acting on the Hilbert space where the *pure* states,

wave-functions, of the system are described. Let us denote by \mathfrak{A} the algebra generated by the observables of the system. In this case, by construction, \mathfrak{A} coincides with the space of bounded operators acting over the Hilbert space \mathfrak{H} , i.e. $\mathfrak{A} = \mathfrak{B}(\mathfrak{H})$.

We will suppose that the system of interest (open or closed) can always be described in terms of a density matrix (also referred to as a statistical operator) ρ . The introduction of the concept of the density matrix is due to Landau [Landau 1927] and von Neumann [von Neumann 1932]⁵. The density matrix must be such that its trace converges to a finite value (which we will take to be normalized to one) and should satisfy the properties of Hermiticity and positivity, viz.⁶:

$$\text{Tr}\{\rho\} = 1, \quad (1.8)$$

$$\rho = \rho^\dagger, \quad (1.9)$$

$$\text{Tr}\left\{\rho A^\dagger A\right\} \geq 0 \quad \forall A \in \mathfrak{A}. \quad (1.10)$$

Following the convention used in the previous section, let us denote the set of all density matrices (the state space) by $S(\mathfrak{A})$ (sometimes, when there is no risk of confusion as to which algebra we are referring to, we will simply use S). As usual, the expectation value of an observable A for a system in the state ρ is defined to be

$$\langle A \rangle_\rho = \text{Tr}\{\rho A\}.$$

Let us mention some of the most interesting properties of the density matrix. First, since the density matrix is Hermitian it can be written in terms of its spectral decomposition (for simplicity we will assume a discrete spectrum):

$$\rho = \sum_i \lambda_i |\lambda_i\rangle\langle\lambda_i|, \quad (1.11)$$

where, using the normalization (1.8), we have that

$$\sum_i \lambda_i = 1, \quad (1.12)$$

$$\langle\lambda_i|\lambda_j\rangle = \delta_{ij}. \quad (1.13)$$

Furthermore, from the positivity condition we know that

$$\lambda_i \geq 0 \quad \forall i.$$

In fact in any representation the diagonal elements of ρ will always be positive semidefinite, i.e. for any complete orthonormal set $\{|n\rangle\}$

$$\rho_{nn} = \langle n|\rho|n\rangle \geq 0 \quad \forall n.$$

⁵As a historical curiosity we would like to mention that the original symbol for the density matrix was different from ρ , the one currently used in the literature. Landau used the letter f , whereas von Neumann used the symbol U which is now usually reserved for unitary operators (the statistical operator is not unitary!)

⁶As is usually done, we will denote the trace of an operator A as $\text{Tr}\{A\}$ (in some, rather old, references this operation is called the spur of A and is denoted as $\text{Sp}\{A\}$, see for example [Yang 62]).

As well, the positivity of ρ imposes certain restrictions on the off-diagonal components ρ_{mn} . Namely, it can be shown that [Blum 1981]

$$|\rho_{mn}|^2 \leq \rho_{mm}\rho_{nn}, \quad (1.14)$$

with equality only occurring if ρ is a pure state (to be defined below).

The positivity condition also implies that the statistical operator ρ can always be written as [Bratelli & Robinson 1987]:

$$\rho = \gamma\gamma^\dagger.$$

The operator γ is not unique, for example a transformation of the form $\gamma \rightarrow \gamma U$, with U a unitary operator, will leave ρ invariant. What is more, γ does not even have to be of the same dimension as ρ . For example, in the finite dimensional case it just needs to have the same numbers of rows [Jaynes 1957].

Another easy to check property of ρ is

$$\text{Tr} \{ \rho^2 \} \leq 1.$$

If we denote the maximum eigenvalue of ρ by $\lambda_{\max} = \max_i \{ \lambda_i \}$, a more accurate bound is

$$\lambda_{\max}^2 \leq \text{Tr} \{ \rho^2 \} \leq \lambda_{\max} \leq 1.$$

Now let us concentrate on a special class of states, namely the *pure* states. We will define a pure state as one that can be described by a state vector $|\psi\rangle$. The density matrix associated with such a state is

$$\rho = |\psi\rangle\langle\psi|. \quad (1.15)$$

From now on we will reserve the symbol ψ to refer to pure states (the only exception to this notation will be in chapter 7, where $\hat{\psi}$ will denote a field operator). Abusing the notation somewhat we will write $\rho = \Psi$ when referring to pure states.

From (1.15) it is obvious that a pure state (normalized to $\langle\psi|\psi\rangle = 1$) satisfies the projection condition

$$\Psi = \Psi^2, \quad (1.16)$$

and therefore it will satisfy

$$\text{Tr} \{ \Psi^2 \} = 1.$$

Also it is easy to see that the spectrum of a pure state will only have one non-zero eigenvalue, which will be equal to one. Hence a condition for purity of a state could be

$$\lambda_{\max} = 1. \quad (1.17)$$

Another interesting property of pure states is that in *any* orthonormal basis $\{|a_i\rangle\}$ the matrix elements of the state satisfy the factorization condition

$$\langle a_m | \Psi | a_n \rangle = c_m \bar{c}_n. \quad (1.18)$$

Which is simply a restatement of the fact that a pure state corresponds to a state vector, in this case with components $c_m = \langle a_m | \psi \rangle$. It is also easy to see from this last equation that a pure state will satisfy the equality relation in (1.14).

1.4 Classical vs. quantum state spaces

In spite of the discussion in section 1.1, it is our opinion that it is safe, no matter what interpretation we chose to follow (except perhaps for some pathological cases we are not aware of), to say that a classical system corresponds to one where all the observables commute. Following the usual convention in the literature we will refer to such an algebra, where all its elements commute amongst themselves, as Abelian. Here we would like to study some of the differences between a quantum state space, one associated with a non-Abelian algebra, and the one associated with an Abelian (classical) algebra.

An important feature of the state space (both in Quantum Theory and classical Statistical Mechanics) is that it is a *convex set*. That is, if $\rho_1, \rho_2 \in S(\mathfrak{A})$ then it is easily verified that

$$\rho = p\rho_1 + (1-p)\rho_2, \quad (1.19)$$

with $p \in [0, 1]$, is also an element of $S(\mathfrak{A})$. From hence forward we will say that a state ρ is a convex combination of the set $\{\rho_\mu\}$ if it can be written as

$$\rho = \sum_{\mu} p_{\mu} \rho_{\mu},$$

with $p_{\mu} \in [0, 1]$ and $\sum_{\mu} p_{\mu} = 1$. If the state cannot be written in this form we will say that it is an *extreme* state. We will denote the set of extreme states as $\partial S(\mathfrak{A})$.

Now let us conduct a small thought experiment. Suppose we measure a certain property, say A , that has N distinct outcomes $\{a_i\}_{i=1}^N$. Let us denote the pure states associated with these outcomes, namely the eigenvectors of A , by $\{\Psi_i^{(A)} = |a_i\rangle\langle a_i|\}_{i=1}^N$ which, by assumption, are orthonormal, i.e.

$$\Psi_i^{(A)} \Psi_j^{(A)} = \Psi_i^{(A)} \delta_{ij},$$

and linearly independent:

$$\sum_i c_i \Psi_i^{(A)} = 0 \quad \Rightarrow \quad c_i = 0 \quad \forall i.$$

That is, the states $\Psi_i^{(A)}$ are extreme states.

Also, as a direct consequence of the orthonormality condition we have that all these states commute amongst themselves:

$$[\Psi_i^{(A)}, \Psi_j^{(A)}] = 0 \quad \forall i, j. \quad (1.20)$$

We will take for granted that the observable A can be written as:

$$A = \sum_i a_i \Psi_i^{(A)}.$$

In a *classical* setting the state space would be formed by all the states constructed as convex combinations of the extreme states corresponding to the pure states, viz:

$$\rho = \sum_i p_i \Psi_i^{(A)},$$

with $\sum_i p_i = 1$.

However, now consider the possibility that there exists another observable, say B , which just as A , results in N distinct outcomes $\{b_i\}_{i=1}^N$ corresponding to the states $\{\Psi_i^{(B)} = |b_i\rangle\langle b_i|\}_{i=1}^N$. Let us assume that B can also be written as:

$$B = \sum_i b_i \Psi_i^{(B)}.$$

It is trivial to show that if $[A, B] = 0$ then both A and B are diagonal in the same basis $\{|a_i\rangle\}$ and hence the set of extreme states of B will coincide with the set of extreme states of A (any good introductory text to Quantum Mechanics will have a proof of this, see for example [Sakurai 1994]).

Now let us assume that B does not commute with A , that is

$$[A, B] \neq 0,$$

then it is plain to see that the states $\{\Psi_i^{(B)}\}$ *cannot* be written as a convex combination of the extreme states $\{\Psi_i^{(A)}\}$. Suppose that there existed a set of coefficients $\{c_{jk}\}$ such that

$$\Psi_j^{(B)} = \sum_k c_{jk} \Psi_k^{(A)}$$

then, using the commutation relations (1.20) we would have that

$$\begin{aligned} [A, B] &= \sum_{ij} a_i b_j [\Psi_i^{(A)}, \Psi_j^{(B)}] \\ &= \sum_{ijk} a_i b_j c_{jk} [\Psi_i^{(A)}, \Psi_k^{(A)}] \\ &= 0 \end{aligned}$$

violating our assumption about the non-commutativity of A and B . In fact, in our proof we did not impose any restriction on the coefficients $\{c_{ik}\}$ (i.e. on whether they belong to a certain interval, real or complex) and hence we can affirm that, in the non-commutative case, none of the extremal states of $S(\mathfrak{A})$ can be expressed as a linear combination of other extremal states. This is just a (important) peculiarity of the space of density matrices, $S(\mathfrak{A})$, as compared to the *superposition principle* on the Hilbert space, \mathfrak{H} , where the linear combination of any combination of state vectors results in another state [Dirac 58].

Furthermore the existence of a single pair of non-commuting observables ensures the existence of an infinity of non-commuting observables as long as one can form observables of the form $C = \alpha A + \beta B$ with $\alpha, \beta \in \mathbb{R}$. This in turn leads us to conclude that for a non-Abelian algebra \mathfrak{A} there exists an uncountable number of extreme states.

It is worth pointing out that although the previous argument is mathematically correct it is possible that not all of these states are physically accessible, as we will see in future chapters.

We have just provided an example of the well known fact that for an Abelian (classical) system the state space is a simplex, that is all the states have a *unique* decomposition in terms of extremal states, whilst in quantum theory this is not so [Bratelli & Robinson 1987] [Streater 1995].

The existence of non-commuting observables implies the existence of an uncountable number of extreme (pure) states that can be used to form an unbounded number of unitarily equivalent basis states, and therefore the decomposition of the non-extremal states is not unique (this property lies at the heart of the well known fact that the correspondence between statistical ensembles and density matrices is infinitely many to one [Hughston *et al.* 1993]). Nonetheless one needs to be careful, for the case of systems with a finite number degrees of freedom the previous statement is true, but systems with an infinite number of degrees of freedom (e.g. in the thermodynamic limit) generally admit several inequivalent irreducible representations (this is especially so in the case of systems which have phase transitions, i.e. systems with broken symmetries and superselection sectors) [Thirring 1981 vol. 3] [Thirring 1983 vol. 4] [Sewell 2002].

An alternative way to show that S for a quantum system is not a simplex is using the superposition principle. In this case, the fact that any superposition of the states $\{|a_i\rangle\}$ is a valid state leads us to conclude that there are several (pure) density matrices that cannot be written as a convex combination of the extremal states $\{|a_i\rangle\langle a_i|\}$ because of the presence of off-diagonal elements ($\langle a_i|\rho|a_j\rangle \neq 0$).

To summarize, we could say that one of the prerequisites to have quantum behaviour is the existence of non-commuting observables (it seems that the superposition principle and non-commutativity principle go hand in hand). As we saw, one of the consequences of this is that in quantum theory the state space is not a simplex, i.e. in a certain way we could say that the quantum state space is more “symmetric” than its classical counterpart. In chapter 7 we will study in more detail this “symmetry” of the quantum state space and show how it is related to the superposition principle. As well, we should (trivially) mention that there are other well known consequences of non-commutativity that distinguish quantum theory from classical mechanics (for example Heisenberg’s uncertainty relations).

1.5 Some definitions of quantumness and classicality

It is now necessary to introduce some criteria to distinguish classical and quantum behaviour. The one predominantly used in this thesis will be the one referred to as *classicality with respect to a partition* which is introduced immediately below. However, for completeness, we will also mention some of the other most often used criterions.

1.5.1 Classicality with respect to partitions

Before introducing a definition of classicality let us just remember that by a *partition* of a Hilbert space one usually understands that one has defined a collection of orthogonal projectors $\{P_\mu\}_\mu$, such that $\sum_\mu P_\mu = \mathbf{1}$ and $P_\mu P_\nu = \delta_{\mu\nu} P_\mu$. If all the projectors are one-dimensional, i.e. $\text{Tr}\{P_\mu\} = 1 \forall \mu$, we will say that the partition is fine-grained. If at least one of the projectors is not one-dimensional, i.e. $\exists \mu$ such that $\text{Tr}\{P_\mu\} > 1$, then we will call the partition coarse-grained.

With these definitions, and following what is usually considered to be classical behaviour in studies of decoherence theory [Zurek 1991] [Giulini *et al.* 1996], let us define classicality as [Scherer *et al.* 2004]:

Definition 1 A state represented by the density operator ρ will be called classical with respect to (w.r.t.) a partition $\{P_\mu\}_\mu$ of the Hilbert space \mathfrak{H} , if

$$\rho = \sum_k p_k \rho_k, \quad \text{where } \forall k \exists \mu \text{ such that } \text{Tr}\{P_\mu \rho_k\} = 1. \quad (1.21)$$

We will denote by $\tilde{C}_{\{P_\mu\}}$ the set of all density operators that are classical w.r.t. the partition $\{P_\mu\}_\mu$ and sometimes we will refer to them as *classical*, or *C*, *states*. As well, it is important to note that this definition allows the possibility of considering certain pure states as classical. The set of extremal (pure) classical states will be denoted by $\partial\tilde{C}_{\{P_\mu\}}$.

The state ρ in definition 1 is assumed to be properly normalized such that $\sum_k p_k = 1$ and $\text{Tr}\{\rho_k\} = 1$. As well, the last statement of the definition means that for every ρ_k in the decomposition there exists a projector $P_\mu \in \{P_\nu\}_\nu$ such that the relationship between their supports is of the form $\text{supp}\{\rho_k\} \subseteq \text{supp}\{P_\mu\}$.

Except where otherwise stated, in this thesis we will suppose that our definitions of classicality are always based on a fine-grained partition. This means that our definition of classicality will in general mean that classical states are diagonal in the representation corresponding to the partition $\{P_\mu\}_\mu$.

An interesting property of our definition of classicality is that, at least for finite dimensional systems, the set $\tilde{C}_{\{P_\mu\}}$ is always non-empty. No matter what our choice of the partition $\{P_\mu\}_\mu$ is, the maximally mixed state $\frac{1}{N}$ will always belong to the set of classical states. In this sense we could think of this state as some sort of centre of the state space $S(\mathfrak{A})$. The existence of the state $\frac{1}{N}$, more than assuring us about the non-emptiness of $\tilde{C}_{\{P_\mu\}}$, guarantees that the intersection of all the possible classical sets is non-empty. Other reasons why $\frac{1}{N}$ can be thought of as a centre of $S(\mathfrak{A})$ will be given in section 5.7.

Given this definition of classical states, we can use its complement in $S(\mathfrak{A})$ to make the definition:

Definition 2 A state represented by the density operator ρ will be called non-classical with respect to (w.r.t.) a partition $\{P_\mu\}_\mu$ of the Hilbert space \mathfrak{H} , if

$$\rho = \sum_k p_k \rho_k + \Pi_Q, \quad \text{where } \Pi_Q \neq 0 \text{ and } \forall k \exists \mu \text{ such that } \text{Tr}\{P_\mu \rho_k\} = 1.$$

The decomposition is chosen such that the Hermitian, and traceless, operator Π_Q has null components along its diagonal ($\forall \mu \quad \text{Tr}\{P_\mu \Pi_Q\} = 0$).

We will denote the set of all these non-classical states by $\tilde{Q}_{\{P_\mu\}}$, and its subset of pure non-classical states by $\partial\tilde{Q}_{\{P_\mu\}}$. Also, sometimes we will refer to the elements of $\tilde{Q}_{\{P_\mu\}}$ as *quantum* or *Q* *states*. Here it is understood that, although all the states ρ considered in this thesis are “quantum” (in the sense that they all correspond to a non-commutative theory), these are the ones that correspond to non-classical behaviour according to our definition. As well, notice that this definition of quantumness can be written as

$$\begin{aligned} \tilde{Q}_{\{P_\mu\}} &= S(\mathfrak{A}) - \tilde{C}_{\{P_\mu\}} \\ &= \left\{ \rho_Q \in S(\mathfrak{A}) \mid \rho_Q = \rho_C + \Pi_Q; \rho_C \in \tilde{C}_{\{P_\mu\}}, \Pi_Q \neq 0 \right\}. \end{aligned}$$

For ρ to represent a proper state (according to conditions 1.8-1.10) the operator Π_Q , besides being Hermitian and traceless, needs to be consistent with the positivity condition (this condition would imply that it is not possible to have the unphysical situation where $(\Pi_Q)_{ij} \neq 0$ if $\rho_{ii} = 0$ or $\rho_{jj} = 0$).

For this definition of quantumness the coherence is characterized by the off-diagonal terms ρ_{mn} (contained in Π_Q). A quantity

$$g_{mn} = \frac{\rho_{mn}}{\sqrt{\rho_{mm}\rho_{nn}}},$$

is a natural measure of the interference contrast and, therefore, of the coherence of the state. In fact, this measure of coherence is, at least from a mathematical point of view, equivalent to Glauber's criterion for first-order coherence in the optical case [Glauber 1963] (this similarity will be explored more in depth in chapter 7).

Because of the relation (1.14), arising from the positivity of ρ , it is easy to see that we do not need to worry about the possibility of g_{mn} diverging since the cases $\rho_{mm} = 0$ or $\rho_{nn} = 0$ imply $\rho_{mn} = 0$ (if ρ is a valid state). Furthermore, the relation (1.14) yields the bound:

$$|g_{mn}| \leq 1.$$

The maximal degree of coherence is characterized by $|g_{mn}| = 1$ and is only achieved if ρ is a pure state.

It is worth noting that, in the case of fine-grained partitions, if $\rho_Q = \rho_C + \Pi_Q$ is a *pure* state (since it yields the same probabilities as ρ_C for the projectors $\{P_\mu = |\mu\rangle\langle\mu|\}$, i.e. $p_\mu = \text{Tr}\{\rho_C |\mu\rangle\langle\mu|\} = \text{Tr}\{\rho_Q |\mu\rangle\langle\mu|\}$) then we must have

$$\Pi_Q = \sum_{\mu \neq \nu} \frac{\sqrt{p_\mu p_\nu}}{\sqrt{\text{Tr}\{|\mu\rangle\langle\mu| \Pi |\nu\rangle\langle\nu| \Pi\}}} |\mu\rangle\langle\mu| \Pi |\nu\rangle\langle\nu|,$$

with $\Pi = |\varphi\rangle\langle\varphi|$ (see section 5.2).

Also let us point out that the definition of quantumness presented here has the useful property that, for any observable, its expectation value can be split as

$$\langle A \rangle_Q = \langle A \rangle_C + \langle A \rangle_\varphi,$$

where $\langle A \rangle_C = \text{Tr}\{\rho_C A\}$ and $\langle A \rangle_\varphi = \text{Tr}\{\Pi_Q A\}$. For example this loosely coincides with what one would expect for the intensity pattern in a double-slit type interference experiment of a “coherent” state, viz:

$$\langle I \rangle = \underbrace{p_1 I_1 + p_2 I_2}_{\langle I \rangle_C} + \underbrace{\sqrt{p_1 I_1 p_2 I_2} \cos \delta}_{\langle I \rangle_\varphi}$$

Thus, at first sight, this definition of classicality (and therefore of quantumness) would appear to be adequate, but one needs to be careful. The decomposition in (1.21) seems to lack the off-diagonal elements associated with the existence of interference effects. Yet having a diagonal ρ by itself does not mean much since ρ is Hermitian and therefore it is always possible to diagonalize

it. Because of this, definition 1 implicitly assumes that the set of projectors $\{P_\mu\}_\mu$ correspond in some sense to those in which the measurement of interest is performed, i.e. to the basis in which one expects to observe, or not, quantum coherence. This renders our definition of classicality into a context dependent property, which is actually both a good and a bad property of our definition. Obviously having a context dependent criterion makes things difficult, and does not coincide with our classical prejudices of dichotomic (yes-no) judgements. But on the other hand it shows that our classicality definition is in some sense compatible with the movable boundary between C and Q within the Copenhagen interpretation.

Under these caveats, a further “classical” characteristic of $\rho_C \in \tilde{C}_{\{P_\mu\}}$ is that in the case of *non-selective projective measurements* compatible with $\{P_\mu\}_\mu$ (described in section 2.1) the state of the system is not perturbed. This is easily seen since

$$\rho_C \xrightarrow{\text{non-selective meas.}} \rho' = \sum_\mu P_\mu \rho_C P_\mu = \rho_C. \quad (1.22)$$

In the next chapter we will study further under what conditions (if any) the definitions 1 and 2 are a suitable criterion of classical and/or quantum behaviour.

1.5.2 Other criteria

The previous criterion of classicality was formulated in terms of states, but we could also use conditions on the observables themselves. For example (as already mentioned in section 1.4) another possible definition of classicality could be the condition that all the observables of the system commute, viz:

$$[A, B] \rightarrow 0 \quad \forall A, B \in \mathfrak{A}, \quad (1.23)$$

where \mathfrak{A} is the algebra generated by the observables of the system. In other words we want the algebra of observables of the system to become Abelian in some proper limit. As we saw in section 1.4 this implies that one no longer would have several equivalent bases to describe the system, which in turn implies that it is no longer possible to realize superpositions of pure states that would result in a new pure state (any combination of pure states would result in a mixture). For the case of ideal decoherence described in section 4.1, and in this case only, the Abelian condition is basically equivalent to the criterion of classicality w.r.t. a partition introduced in the previous section.

In most cases this criterion would also be equivalent to the usual correspondence limit condition, $\hbar \rightarrow 0$, since the commutators of most canonical observables are proportional to \hbar . In fact several models are built such that they will correspond to a classical model in the limit $\hbar \rightarrow 0$ (Bohr’s correspondence principle). This is especially true in quantum field theories where one starts from a classical Lagrangian which is later quantized. However, it is worth noting that this correspondence limit runs into troubles when studying systems that in the classical limit are (or should be) chaotic [Bhattacharya *et al.* 2004] [Zurek 2003]. (In fact, it is our opinion that this problem has been known to exist, in a different guise, since the 1950’s when [Wigner 1950] found that the commutation relations are not determined uniquely by the equations of motion; even if the form of the Hamiltonian is fixed).

As well, we could relax the previous condition of commutativity, and simply require that the fluctuations of the relevant observables be negligible. That is,

$$\frac{\Delta A}{\langle A \rangle} \rightarrow 0, \quad (1.24)$$

in some suitable limit ($\Delta A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$). In this case one could expect that in general there would be very small deviations from the expected value, and from Ehrenfest's theorem the classical equations of motion should apply to the observable A . Obviously this criterion is related to the Abelian condition because of Heisenberg's uncertainty relations. This criterion of negligible fluctuations has been studied for systems in the thermodynamic limit by [Frasca 2003] but we will not pursue it further.

An alternative criterion for states, frequently used when dealing with systems with continuous degrees of freedom, is to study the Wigner function $W(x, p)$ [Feynman 1972], which is basically a modified Fourier transform of the density matrix, viz:

$$W(x, p) = \int d\eta \, e^{-ip\eta/\hbar} \rho\left(x + \frac{\eta}{2}, x - \frac{\eta}{2}\right).$$

In this case classical behaviour is taken to be equal to a non-negative Wigner function over the whole of phase space [Giulini *et al.* 1996].

Although each of these criteria have their own merits, for reasons of practicality, and because we have chosen to work in the Schrödinger picture, we will only study the criterion of classicality w.r.t. a partition (the only exception will be in chapter 7).

Chapter 2

Observing Quantum Coherence

In this chapter we would like to address some of the issues related to characterizing and observing quantum behaviour. The first section introduces the basic terminology related to measurements that will be used throughout the thesis. Sections 2.2 through 2.4 study the Wigner-Araki-Yanase theorem, and its relation to weak measurement and postselection. Finally, in sections 2.5 and 2.6 we study some of the problems related to observing quantum behaviour (as defined in section 1.5.1) and the ambiguities associated to our definitions of classicality and quantumness.

2.1 Measurements

To avoid any misunderstandings in future sections we would like to introduce here some standard terminology related to quantum measurements.

In the standard interpretation of Quantum Theory, measurements are described by a collection $\{M_\mu\}$ of *measurement operators* [Kraus 1983]. The index μ refers to the measurement outcomes that may occur in the experiment. If the state of the system is described by ρ immediately before the measurement then the probability that the result μ occurs is given by

$$p(\mu) = \text{Tr} \left\{ M_\mu^\dagger M_\mu \rho \right\}. \quad (2.1)$$

If outcome μ is registered, then the state of the system immediately after the measurement is

$$\rho'_\mu = \frac{M_\mu \rho M_\mu^\dagger}{\text{Tr} \left\{ M_\mu^\dagger M_\mu \rho \right\}}. \quad (2.2)$$

The measurement operators satisfy the *completeness equation*

$$\sum_\mu M_\mu^\dagger M_\mu = \mathbf{1}, \quad (2.3)$$

this ensures that the probabilities $p(\mu)$ are normalized to 1.

Most elementary books on Quantum Mechanics only consider the case where the measurement operators correspond to orthogonal projectors, we will refer to these as projective, or orthogonal, measurements. The slight generalization of the measurement postulate presented here, where the measurement operators are not necessarily projectors, is called a positive operator-valued measurement (POVM).

The measurement of the collection $\{M_\mu\}$ will lead to a decomposition of the ensemble into various sub-ensembles labelled by the index μ . Such a splitting of the original ensemble into various ensembles, each conditioned on a specific measurement outcome will be referred to as a *selective measurement*.

One could also imagine an experimental situation where all the outcomes of the measurement are mixed once again according to the probabilities $p(\mu)$. The resulting ensemble would then be described by

$$\rho' = \sum_{\mu} p(\mu) \rho'_\mu = \sum_{\mu} M_\mu \rho M_\mu^\dagger. \quad (2.4)$$

This mixing of the sub-ensembles after measurement is referred to as *non-selective measurement*.

The previous represents a general set of rules (postulates) for the calculation of the probability of a certain event and for the state of the system after a measurement. However, it does not give us a description of the mechanism behind the measurement process itself. The archetypical (unitary) model of the measurement process, originally due to [von Neumann 1932], consists in supposing that the system, initially in the pure state $|\psi\rangle_S = \sum_n c_n |n\rangle_S$, interacts with the measurement apparatus, initially prepared in the state $|m_0\rangle_M$, in such a way that the state is transformed as:

$$|\psi\rangle_S |m_0\rangle_M \xrightarrow{U} |\Phi\rangle = \sum_n c_n |n\rangle_S |m_n\rangle_M. \quad (2.5)$$

If the measuring apparatus states are orthonormal, i.e. $\langle m_i | m_j \rangle = \delta_{ij}$, the measurement is called *ideal* or *strong*. It is also worthwhile to consider the case where the apparatus states are not orthogonal, we will refer to this case as *non-ideal* or *weak*. Nonetheless, notice that for the process to be considered as a measurement the apparatus states need to be distinguishable. Therefore we will require that $\langle m_i | m_j \rangle \neq 1$ whenever $i \neq j$. In what follows we will refer to $|\Phi\rangle$ as the *premeasurement state*.

The typical example of a Hamiltonian resulting in this type of evolution is

$$H_{int} = \sum_n |n\rangle_S \langle n| \otimes B_n^M,$$

where $B_n^M = (B_n^M)^\dagger$ are operators of the measuring apparatus, and H_{int} is the interaction term in the Hamiltonian of the composite system $H_{SUA} = H_S + H_M + H_{int}$.

The resulting apparatus states $|a_n\rangle$ are generally called “pointer states”. However, this name is misleading because, due to the superposition principle, the decomposition of $|\Phi\rangle$ on the rhs of (2.5) is not unique. This is part of the so-called “quantum measurement problem” (for an introductory presentation see Zeh’s contribution in [Giulini *et al.* 1996]. A nice presentation of the bizarre consequences of this measurement problem when applying Quantum Mechanics to macroscopic bodies can be found in [Leggett 1984]). In spite of this, the formation of correlations in (2.5) is considered to be the “first step” of the measurement process in most descriptions. The general approach then has been to explain why a particular pointer basis dominates over the other ones and on the collapse of the wave-function (the selection of a particular outcome in 2.5). This is the other main component of the “quantum measurement problem”. For a review of the most recent approaches to the resolution of this problem we refer the reader to [Schlosshauer 2004]; a collection of the main early contributions to this subject can be found in [Wheeler & Zurek 1983].

As it is surely well known to the reader the “quantum measurement problem” is a highly debated topic open to a lot of speculation. However, in this thesis we do not want to risk incurring in the all too common speculations surrounding this subject. Instead our approach will be to accept what could be considered to be some of the mainstream interpretations and then analyse what are the consequences of these under various conditions. In particular, as regards equation (2.5), we will adhere to what could broadly be called the Copenhagen interpretation [Stapp 1972] [Bub 1997], and we will accept that it provides a correct description of the (indirect) measurement when it is complemented by a non-unitary process resulting in the so-called collapse of the wave-function.

2.2 WAY theorem

Before continuing let us recall a theorem due to Wigner, Araki and Yanase that restricts the observables that can be measured in certain type of measurements when there exists a globally conserved quantity [Wigner 1952] [Araki & Yanase 1960]. The theorem runs as follows:

Suppose there exists an additive physical quantity, of the system (S) and measuring apparatus (M), of the form

$$Q = Q^S \otimes \mathbf{1} + \mathbf{1} \otimes Q^M$$

that is globally conserved, i.e.

$$[U_t; Q] = 0 \quad \forall t.$$

Then the Wigner-Araki-Yanase (WAY) theorem states that M *cannot* measure any quantity A of S that does not commute with Q^S when an ideal strong von Neumann measurement is performed (see previous section) [Wigner 1952] [Araki & Yanase 1960]. Nonetheless, the theorem is not completely robust and when certain types of errors are allowed it need no longer hold [Yanase 1961] [Ghirardi *et al.* 1981a].

Let us explore further the validity of the WAY theorem in the case of non-ideal measurements. In particular, we will prove that the theorem still holds in the case of non-orthogonal pointer states of the measuring apparatus :

Let $\{|a_n\rangle\}$ be a complete orthonormal set of eigenstates of the observable A of the system S , and let $|m_0\rangle$ be the reference (“zero”) state of the measuring apparatus M . In the ideal von Neumann measurement the process is driven by a unitary evolution operator U which generates the premeasurement entanglement $U|a_n\rangle|m_0\rangle = |a_n\rangle|m_n\rangle$, where the measuring apparatus’ states $\{|m_n\rangle\}$ are normalized to one and in the ideal case the pointer states are orthogonal $\langle m_i|m_j\rangle = \delta_{ij}$. However, let us omit the orthogonality condition and only require that the pointer states satisfy $\langle m_i|m_j\rangle \neq 1$ whenever $a_i \neq a_j$ (otherwise there would be no measurement, see discussion in previous section). By hypothesis Q is a conserved quantity and therefore $[U, Q] = 0$, or equivalently $Q = U^\dagger Q U$.

Now for the proof. For any pair $a_i \neq a_j$ ($\langle a_i|a_j\rangle = 0$) it is easy to see that the following holds:

$$\begin{aligned}
\langle a_i | Q^S | a_j \rangle &= \langle a_i | \langle m_0 | Q | a_j \rangle | m_0 \rangle \\
&= \langle a_i | \langle m_0 | U^\dagger Q U | a_j \rangle | m_0 \rangle \\
&= \langle a_i | \langle m_i | Q | a_j \rangle | m_j \rangle \\
&= \langle a_i | \langle m_i | Q^S \otimes \mathbf{1} + \mathbf{1} \otimes Q^M | a_j \rangle | m_j \rangle \\
&= \langle a_i | Q^S | a_j \rangle \langle m_i | m_j \rangle
\end{aligned} \tag{2.6}$$

But, since by hypothesis $\langle m_i | m_j \rangle \neq 1$, the only way this can be satisfied is if

$$\langle a_i | Q^S | a_j \rangle = 0 \quad \forall a_i \neq a_j$$

That is, Q^S must be diagonal in the basis $\{|a_n\rangle\}$ which in turn implies that $[Q^S, A] = 0$. QED.

The proof given above is a very slight generalization of the one given in [Ghirardi *et al.* 1981a] (which assumes that $\langle m_i | m_j \rangle = 0$). In fact, our modification is so trivial that we cannot claim it as a new result. However, what we believe to be new, is the realization that by relaxing the conditions so as to include the possibility of uncertain distinguishability of the apparatus states, i.e. $\langle m_i | m_j \rangle \neq 0$, the domain of validity of the WAY theorem extends to the case of *weak measurements* as described in [Aharonov *et al.* 1988] and [Duck *et al.* 1989]. Therefore its associated limitations should be taken into account for these measurements, in particular when studying the extreme events predicted when weak measurements are coupled with postselection (see section 2.4).

As mentioned above, in spite of the previous analysis, it can be shown that the WAY theorem can be overcome when one considers more general errors of the type [Yanase 1961] [Ghirardi *et al.* 1981a]:

$$U |a_n\rangle |m_o\rangle = \sqrt{1-\delta} |a_n\rangle |m_n\rangle + \sqrt{\delta} |a_{n\perp}\rangle |m_{n\perp}\rangle \tag{2.7}$$

(with $\langle a_n | a_{n\perp} \rangle = 0$). The minimum size of the error required to overcome the WAY restriction depends on the experimental situation. Qualitatively, the “larger” the measuring apparatus is (i.e. the greater its contribution to the value of the conserved quantity) the smaller the required error is. For example, if we consider a measurement of the z -component of the spin of a spin- $\frac{1}{2}$ particle, and if one assumes that the total angular momentum of the particle and the measurement apparatus is conserved, then the minimal error is

$$2\delta \geq \min_{i=x,y} \left\{ \frac{\hbar^2}{8 \langle m_0 | L_i | m_0 \rangle} \right\} \tag{2.8}$$

where L_i , $i = x, y$, corresponds to the angular momentum of the measuring apparatus.

In the context of this thesis we are interested in this theorem because, at least in principle, it has the potential to limit the observables that can be measured and hence the basis in which we could be interested to study decoherence and recoherence. However, the extended validity of the WAY theorem to the case of weak measurements also leads us to question what would be the implications of considering errors of the type of equation (2.7) on the peculiar results obtained when weak measurements are coupled to post-selection [Aharonov *et al.* 1988] [Duck *et al.* 1989]. This will be done in the next sections.

2.3 Misalignment errors

Given the results of the previous section, here we will analyse what are some of the effects of considering errors of the general form of those in equation (2.7). In particular, we will develop a model for these errors that we will be able to use later when studying the consequences of these errors when coupled to post-selection.

For simplicity let us concentrate on the measurement of an observable A with only two non-degenerate eigenvalues denoted by a_{\pm} and eigenvectors $|\pm\rangle$. Then suppose that the premeasurement interaction between the system and the reference state of the measuring apparatus has the following action:

$$|\pm\rangle |m_o\rangle \xrightarrow{U} |\pm\rangle |\eta_{\pm}\rangle + |\mp\rangle |\varepsilon_{\pm}\rangle.$$

From now on we will refer to this type of errors as *misalignment errors*. In this expression the pointer states $|\varepsilon_{\pm}\rangle$ and $|\eta_{\pm}\rangle$ are *not* normalized. In fact, if this misaligned state is truly the result of a unitary interaction between the reference pointer state and an arbitrary initial state of the system, then we have the restrictions:

$$\langle\eta_{\pm}|\eta_{\pm}\rangle + \langle\varepsilon_{\pm}|\varepsilon_{\pm}\rangle = 1, \quad (2.9)$$

and

$$\langle\eta_{+}|\varepsilon_{-}\rangle = -\langle\varepsilon_{+}|\eta_{-}\rangle. \quad (2.10)$$

If the initial state of the system is given by $|\psi_{in}\rangle = \alpha_{+}|+\rangle + \alpha_{-}|-\rangle$, with $|\alpha_{+}|^2 + |\alpha_{-}|^2 = 1$, the state of the system plus apparatus after the measurement interaction will be:

$$|\Phi^{SM}\rangle = \alpha_{+}(|+\rangle|\eta_{+}\rangle + |-\rangle|\varepsilon_{+}\rangle) + \alpha_{-}(|-\rangle|\eta_{-}\rangle + |+\rangle|\varepsilon_{-}\rangle). \quad (2.11)$$

If we trace out the degrees of freedom of the system, the state of the measuring apparatus is given by the mixed state:

$$\rho_M = |M_{+}\rangle\langle M_{+}| + |M_{-}\rangle\langle M_{-}|, \quad (2.12)$$

where

$$|M_{\pm}\rangle = \alpha_{\pm}|\eta_{\pm}\rangle + \alpha_{\mp}|\varepsilon_{\mp}\rangle.$$

Then it is obvious that in the case of a misalignment error the state of the pointer variable apart from “measuring” the amplitudes $|\alpha_{\pm}|$, as occurs in an ideal or weak measurement, also has the potential of being modified by the relative phase $\theta := \arg\{\alpha_{+}\alpha_{-}^{*}\}$.

To make the previous point clearer let us make some specific assumptions about the pointer states after the measurement interaction. Consider the case where the pointer variable corresponds to a continuous degree of freedom, in particular the pointer corresponds to a generalized momentum coordinate of the “measuring” device. Then, a choice consistent with the restrictions (2.9) and (2.10) could be

$$|\eta_{\pm}\rangle = \sqrt{1-\delta}|G_{\pm}(\Delta_{\eta})\rangle, \quad (2.13)$$

and

$$|\varepsilon_{\pm}\rangle = \pm\sqrt{\delta}e^{\pm i\epsilon}|G_{\mp}(\Delta_{\varepsilon})\rangle. \quad (2.14)$$

To maintain our interpretation of this process as a type of error we will require that $\delta \leq 1/2$. Also, if we want to use this type of error to circumvent the WAY theorem then there exists a minimum

value for δ determined by the initial state of the pointer (see equation 2.8) [Ghirardi *et al.* 1981a]. The states $|G_{\pm}(\Delta_x)\rangle$, $x = \eta, \varepsilon$, are normalized to one, and we choose them to be Gaussian wavefunctions which in the momentum representation are centred around the eigenvalues of A . These can be written as:

$$|G_{\pm}(\Delta_x)\rangle = \int dp G_{\pm}(p, \Delta_x) |p\rangle, \quad (2.15)$$

with

$$G_{\pm}(p, \Delta_x) = \sqrt{\frac{2\Delta_x}{\sqrt{2\pi}}} \exp\left\{-\Delta_x^2 (p - a_{\pm})^2\right\}$$

Then, the probability distribution of the pointer variable after the misaligned measurement would be given by (to ease the notation we will write $G_{\pm}(p, \Delta_x)$ as $G_{\pm x}$):

$$\begin{aligned} P(p) = & |\alpha_+|^2 ((1-\delta) G_{+\eta}^2 + \delta G_{-\varepsilon}^2) + \\ & |\alpha_-|^2 ((1-\delta) G_{-\eta}^2 + \delta G_{+\varepsilon}^2) + \\ & 2|\alpha_+\alpha_-| \sqrt{\delta(1-\delta)} \cos\{\theta + \epsilon\} (G_{-\eta}G_{-\varepsilon} - G_{+\eta}G_{+\varepsilon}). \end{aligned}$$

The effect of our misalignment error becomes clearer. Suppose the initial state of the system is $|+\rangle$ and the pointer states have a small momentum uncertainty (i.e. a large value of Δ) compared to $|a_+ - a_-|$. It follows that the distribution consists of two “spikes”, the larger one centred around the “correct” eigenvalue a_+ , whilst the other one is centred on the “incorrect” value a_- . Furthermore, for states with $|\alpha_+| \neq 1$ the distribution of pointer values will depend on the relative phase $\theta = \arg\{\alpha_+\alpha_-^*\}$. Both of these properties justify our term “misalignment error” since it is similar to the type of behaviour we would expect from a slight misalignment of the magnet or polarizer in a Stern-Gerlach or optical experiment.

To further clarify the situation let us consider the limiting case where $\Delta_{\eta} = \Delta_{\varepsilon} (= \Delta)$. In this case the picture is greatly simplified if we define the unitary operator of the system

$$E = \sqrt{1-\delta} 1_S + \sqrt{\delta} D,$$

where D is another unitary operator given by

$$D = e^{i\epsilon} |-\rangle\langle +| - e^{-i\epsilon} |+\rangle\langle -|.$$

Then the whole pre-measurement (entangling) process leading to the system-apparatus state in equation (2.11) can be modelled as:

$$|\Phi^{SM}\rangle = e^{iqA} (E \otimes 1_M) |\psi_{in}\rangle |G_0(\Delta)\rangle, \quad (2.16)$$

with $|G_0(\Delta)\rangle$ being equal to the Gaussian wavefunction defined in (2.15) but centred at $p = 0$, and q the conjugate variable of p , i.e. $[q, p] = i1_M$.

Thus, in this particular case the effect of the misalignment error is obvious. The pointer variable instead of interacting with $|\psi_{in}\rangle$ interacts with the rotated state $E|\psi_{in}\rangle$. However this “rotation” cannot be represented as the result of a measurement interaction e^{iBq} , with B an observable satisfying $[A, B] \neq 0$ (Actually this can be approximately the case if one has $\Delta \ll 1$,

but in general it is not true). This rotation can be better understood if we consider the case where the initial state is given by the superposition

$$|\psi_{in}^+\rangle = \sqrt{1-\delta}|+\rangle - \sqrt{\delta}e^{i\epsilon}|-\rangle, \quad (2.17)$$

then

$$e^{iqA}(E \otimes 1_M)|\psi_{in}^+\rangle|G_0(\Delta)\rangle = |+\rangle|G_+(\Delta)\rangle.$$

Thus, for the measurement to result in a single spike (which in the error-free case would be interpreted as the state being in the state $|+\rangle$), the incoming state has to be in the superposed state (2.17).

If we return to the general case where $\Delta_\eta \neq \Delta_\epsilon$, and we introduce the parameter $k := \sqrt{\frac{2\Delta_\eta\Delta_\epsilon}{(\Delta_\eta^2 + \Delta_\epsilon^2)}}$, from the $P(p)$ distribution we can easily calculate the mean value of the pointer variable to be:

$$\begin{aligned} \langle p \rangle_{\rho_M} = & a_+ \left(|\alpha_+|^2 (1-\delta) + |a_-|^2 - 2k|\alpha_+\alpha_-| \sqrt{\delta(1-\delta)} \cos\{\theta + \epsilon\} \right) + \\ & a_- \left(|\alpha_-|^2 (1-\delta) + |a_+|^2 + 2k|\alpha_+\alpha_-| \sqrt{\delta(1-\delta)} \cos\{\theta + \epsilon\} \right) \end{aligned} \quad (2.18)$$

Although having $\Delta_\eta \neq \Delta_\epsilon$ can result in very exotic behaviour for the distribution $P(p)$, it is easy to convince oneself that $k \leq 1$ for any value of Δ_η and Δ_ϵ . Hence, one always has that the mean value of the pointer's momentum will be bounded by the eigenvalues of A , viz. $\langle p \rangle_{\rho_M} \in [a_-, a_+]$. As we will see in the next section this is not always the case when one considers post-selections of the state of the system.

Before continuing we must caution the reader to take our model of misalignment errors with a rather large pinch of salt as regards the WAY theorem. For example, if the globally conserved variable is the total angular momentum, which would be the most obvious choice if we applied the previous scheme to spin- $\frac{1}{2}$ particle, then our model does not serve to overcome the WAY theorem. In fact our model does not even conserve the z-component of the total angular momentum, $\frac{1}{2}\hbar\sigma_z + L_z$ (where L_z is the z-component of the angular momentum $L = \vec{r} \times \vec{p}$ of the probe); whereas the error-free case does at least conserve this component (but not the others). The reason for our choice of model lies in the application given to it in the next section to the case of extreme values obtained when the scheme is coupled to post-selection. The problem is that the only tractable example we know of a model satisfying the WAY theorem for this conserved quantity, given in [Ghirardi *et al.* 1981b], is not suitable for this purpose since the probe is limited to a discrete spectrum with only three eigenvalues (the reason why this is not suitable for our purposes will become clear in the next section).

2.4 Misalignments and post-selection

As shown by Aharonov, Albert and Vaidman (AAV) [Aharonov *et al.* 1988], and then clarified by Sudarshan *et al.* [Duck *et al.* 1989], some very interesting effects can arise when one considers weak measurements (non-orthogonal pointer states) coupled to post-selection of the quantum state of the system. Namely, for certain choices of the initial state of the system, $|\psi_{in}\rangle$, and of the post-selected state, $|\psi_f\rangle$, one can obtain states of the pointer variable whose mean values lie

well outside the spectrum of the *a priori* measured observable A . However, as we saw in section 2.2, weak measurements are subject to the restrictions of the WAY theorem and here we would like to consider what are the implications of the errors needed to overcome these restrictions. We will concentrate on the example of a two-level system and on the misalignment errors of the previous section.

Let us start from the state of the system plus apparatus $|\Phi^{SM}\rangle$, given in equation (2.11), resulting from the misaligned measurement of an observable A . Immediately after this measurement we perform another, *projective*, measurement of some other observable B and we select a single outcome. This puts the quantum system into the definite final state:

$$|\psi_f\rangle = \beta_+ |+\rangle + \beta_- |-\rangle.$$

After this post-selection the pointer variable is left in the state

$$\rho_M^{P-S} = \text{Tr}_S \{ (|\psi_f\rangle\langle\psi_f| \otimes 1) |\Phi^{SM}\rangle\langle\Phi^{SM}| \},$$

which, up to a normalization constant of $1/\text{Tr} \{ \rho_M^{P-S} \}$, corresponds to the pure state:

$$|\varphi_M^{P-S}\rangle = \beta_+^* \alpha_+ |\eta_+\rangle + \beta_-^* \alpha_- |\eta_-\rangle + \beta_+^* \alpha_- |\varepsilon_-\rangle + \beta_-^* \alpha_+ |\varepsilon_+\rangle. \quad (2.19)$$

AAV's point is that when one considers an “ideal weak measurement” (without the $|\varepsilon_\pm\rangle$ terms) with Gaussian wavefunctions for the pointer momentum, then under certain conditions this can yield mean values $\langle p \rangle_{\varphi_M^{P-S}}$ well outside the spectrum of A . In fact for a restricted set of conditions the mean value will coincide with the quantity

$$A_w = \frac{\langle\psi_f|A|\psi_{in}\rangle}{\langle\psi_f|\psi_{in}\rangle}$$

which they call the *weak value of A*.

To better compare our example with misalignment errors to AAV's results let us concentrate in the case where the pointer wavefunctions $|\eta_\pm\rangle$ and $|\varepsilon_\pm\rangle$ are given by the Gaussian wavefunctions in equations (2.13) and (2.14). Furthermore let us restrict ourselves to the range of conditions where AAV's Gaussian approximation holds, viz. [Duck *et al.* 1989]:

$$\Delta_\eta \ll 1/A_w$$

and

$$\Delta_\eta \ll \min_{n=2,3,\dots} \left| \frac{\langle\psi_f|A|\psi_{in}\rangle}{\langle\psi_f|A^n|\psi_{in}\rangle} \right|^{\frac{1}{n-1}}$$

In this case the wavefunction of the pointer variable in the p -representation, up to a normalization constant, is given by:

$$\begin{aligned} \varphi_M^{P-S}(p) &= \sqrt{1 - \delta N_\eta} \langle\psi_f|\psi_{in}\rangle \exp \left\{ -\Delta_\eta^2 (p - A_w)^2 \right\} + \\ &\quad \sqrt{\delta} \left(\beta_-^* \alpha_+ e^{i\varepsilon} G_-(p, \Delta_\varepsilon) - \beta_+^* \alpha_- e^{-i\varepsilon} G_+(p, \Delta_\varepsilon) \right), \end{aligned} \quad (2.20)$$

where $N_\eta = \sqrt{2\Delta_\eta/\sqrt{2\pi}}$. As expected, when $\delta = 0$ this wavefunction coincides with AAV's results.

Although in the previous example it is evident that the presence of errors can have a significant effect on AAV's results it is still not clear what is the exact way in which these are altered. To better understand this let us consider the limiting case when $\Delta_\eta = \Delta_\epsilon$ ($:= \Delta$). As we saw in the previous section, in this case the calculations are greatly simplified and some simple algebra shows that, up to a normalization constant, the approximate state of the pointer variable in the p -representation, will be:

$$\varphi_M^{P-S}(p) = \langle \psi_f | E | \psi_{in} \rangle \exp \left\{ -\Delta^2 (p - A_{error})^2 \right\}. \quad (2.21)$$

Where we have introduced the quantity

$$A_{error}(\delta, \epsilon) = \frac{\langle \psi_f | AE | \psi_{in} \rangle}{\langle \psi_f | E | \psi_{in} \rangle}. \quad (2.22)$$

If we suppose that the spread of q values is governed by Δ this approximation is valid whenever:

$$\Delta \ll 1/A_{error} \quad (2.23)$$

and

$$\Delta \ll \min_{n=2,3,\dots} \left| \frac{\langle \psi_f | AE | \psi_{in} \rangle}{\langle \psi_f | A^n E | \psi_{in} \rangle} \right|^{\frac{1}{n-1}}. \quad (2.24)$$

These results, where $\Delta = \Delta_\eta = \Delta_\epsilon$, coincide with the comments of the previous section. As expected, the presence of a misalignment error translates to a dependence of the “weak value”, and its range of validity, on the rotated state $E |\psi_{in}\rangle$ instead of $|\psi_{in}\rangle$.

Thus, for this simplified type of errors, the conclusions of [Aharonov *et al.* 1988] and [Duck *et al.* 1989] remain valid *mutatis mutandis*. However, it is worth pointing out that the extreme values predicted by AAV depend on particular combinations of $|\psi_{in}\rangle$ and $|\psi_f\rangle$, and therefore the modification $E |\psi_{in}\rangle$ would change the location of the peculiar effects.

As regards the WAY theorem we must note that the measurement Hamiltonian used in the spin- $\frac{1}{2}$ examples of [Aharonov *et al.* 1988] and [Duck *et al.* 1989] does not conserve the total angular momentum of the spin and the pointer variable (its momentum), only the z -component is conserved. If we accept this lack of conservation as valid then its results are compatible with the WAY theorem as they stand. If not, if we insist that in the physical situation there exist some other conserved quantities, we will have to consider the effect of errors of the type presented here. However, we must emphasize once again that our particular model of misalignment errors is just of the general form of the errors necessary to by-pass the WAY theorem (as well we have ignored the implications of the WAY theorem on the postselection process). For the concrete case where the global conserved quantity is the total angular momentum our misalignment error is still not a proper solution against the limitations imposed by the WAY theorem. This remains an open problem (a possible direction, though mathematically complicated, could be to modify the example in [Ghirardi *et al.* 1981b], that does solve the WAY theorem in this case, such that their probe admits a broader range of outcomes -in their example the probe only allows for three possible outcomes). Nevertheless, we know that there must be systems where AAV's conclusions

remain valid since, at least for the case of optical systems, these have been experimentally verified [Ritchie *et al.* 1991].

Lastly, although the extreme movements of the pointer variable have been verified to take place, we would like to express our scepticism of the interpretation of these as a measurement of the properties of the “measured” system. For example, if one were actually to observe the claim in the title of AAV’s original article (“How the Result of a Measurement of a Component of the Spin of a Spin- $\frac{1}{2}$ Particle Can Turn Out to be 100”), would the nature of the measured particle switch from a fermion to a boson because of the post-selection procedure?

2.5 Known unknowns and unknown unknowns (or *Rumsfeld’s* take on Quantum Mechanics)

In the immortal words of Donald Rumsfeld (U.S. Secretary of Defense) talking on the threats of terrorism (from a neoconservative point of view):

“As we know, there are known knowns; there are things we know we know. We also know there are known unknowns; that is to say we know there are some things we do not know. But there are also unknown unknowns - the ones we don’t know we don’t know”.

Let us first point out that if we were to accept the possibility of the existence of certain *unknown unknowns*, e.g. hidden variables, then our whole discussion about making a distinction between quantum and classical behaviour risks becoming irrelevant (by rendering the system always classical). However, we will accept the validity of the Bell theorem [Bell 1987], and its experimental verifications (one of the more recent reports of this can be found in [Rowe *et al.* 2001]). Thus, we will assume that no such (local) hidden variables exist, and if they did they would still result in a non-classical theory. Therefore (doing quite the opposite to Rumsfeld’s politics) we will ignore these unknown unknowns, and take for granted that one of our *known knowns* will be that we can associate with the system at least one pair of non-commuting observables.

Given our previous assumption, it is important to notice that the main conceptual precept behind the definition of classicality w.r.t. a partition $\{P_n\}$ (as defined in section 1.5.1) is that it supposes the existence of certain preferred *known unknowns* of the form $A = \sum a_i |a_i\rangle\langle a_i|$ (which for simplicity we will assume to be non-degenerate) that are used to define the basis in which classicality will be defined, e.g. $P_n = |a_n\rangle\langle a_n|$. The problem with this is that no measurement of these observables will yield any information on the off-diagonal components used to distinguish the sets $\tilde{C}_{\{P_n\}}$ and $\tilde{Q}_{\{P_n\}}$. The measurement of this observable, and any other compatible with it, will only yield information about the diagonal components of the state ρ . Therefore, to make any distinction, we must also have access to certain incompatible *known unknowns* B such that $[A, B] \neq 0$. However, as is well known, these observables cannot be simultaneously measured for a single copy of the system, and if we want to make a judgement on the quantumness or classicality of the system we will need access to multiple identically prepared copies. Only then will it be possible to reconstruct the statistical operator ρ , and then make some decision (for some of the standard statistical techniques to accomplish the reconstruction we recommend [Helstrom 1976]).

Nevertheless, we would like to stress that the definition of classicality with respect to a certain partition is not foolproof. Consider the archetypical example of a double slit experiment [Feynman 1965]. The interference pattern observed at the screen, associated with the coherent superposition of both possibilities, is usually considered to be proportional to the distribution

$$|\psi(x)|^2 = p_1 |\psi_1(x)|^2 + p_2 |\psi_2(x)|^2 + 2\sqrt{p_1 p_2} |\psi_1(x)| |\psi_2(x)| \cos\{\delta(x)\}$$

In this case, for most interpretations of Quantum Mechanics, it is obvious that the system is behaving in the quantum regime. After all we have the conspicuous interference term $\cos\{\delta(x)\}$ which is one of the main features of quantum behaviour. Thus, it would be only natural to define classicality with respect to the configuration basis, i.e. $P_x \sim |x\rangle\langle x|$, and classify the system as belonging to the set of non-classical states \tilde{Q} . However, notice that this probability density would be encoded in the diagonal elements of the density matrix $\rho(x, x')$, i.e. in the diagonal elements of the basis with respect to which classicality is defined. Thus, we have an example where we could decide whether the system is Q or C simply from the information contained in the diagonal elements of the density matrix.

Also, it is worth remembering that if the measurement process suffers from misalignment errors (as described in section 2.3) then a measurement of a “classical” observable, one diagonal in the basis defined by the partition used for classicality, will depend on the off-diagonal components of ρ .

The double slit experiment also opens the door to another well known problem, mainly the one of the choice of the observer. For example, for a given free particle (and a fixed distance between the slits and the detection screen), the existence of interference fringes will depend crucially on the relation between the wavelength of the particle and the separation between the slits. The latter is arguably a parameter freely chosen by the observer. Thus, whether or not interference (quantumness) is observed will depend on the choice of the observer (and his, or her, experimental abilities).

A clear, and recent, example of the rôle of the choices of the observer is the case of fullerene molecules. In a series of beautiful experiments conducted by Zeilinger’s group they have observed interference effects of these molecules in matter wave interferometers [Arndt *et al.* 1999] [Hackermüller *et al.* 2004]. However, it is also possible to observe these molecules as well-localized objects (see for example [Goel *et al.* 2004] for some high resolution electron transmission microscopy images of C_{60} molecules). Loosely, these two different examples show also how a quantumness criterion depends on whether one is performing a coarse-grained or a fine-grained description.

In the next section we will analyse a criterion for the compatibility of the descriptions of two observers, and see how it relates to the definition of classicality with respect to a partition.

2.6 Compatibility of Q-C assignments between observers

Following the last comment in the previous section let us study under what conditions can two observers agree on whether a system is behaving C or Q as regards the definition of classicality w.r.t. a partition $\{P_\mu\}$ given in section 1.5.1. For this purpose we will use a set of criteria, derived by Brun, Finkelstein, and Mermin (BFM) [Brun *et al.* 2002], for the compatibility between the state assignments, ρ_A and ρ_B , of two different observers, Alice and Bob, describing one and the same system.

The first, which we will call the *first BFM condition* (BFM-1), states that ρ_A and ρ_B are compatible if and only if:

$$\text{supp}\{\rho_A\} \cap \text{supp}\{\rho_B\} \neq \emptyset,$$

or equivalently

$$\dim\{\text{supp}\{\rho_A\} \cap \text{supp}\{\rho_B\}\} \geq 1.$$

($\text{supp}\{M\}$ denotes the support of the operator $M \in \mathfrak{B}(\mathfrak{H})$ which is defined to be the subspace of \mathfrak{H} spanned by the eigenvectors of M corresponding to nonzero eigenvalues).

The *second BFM condition* (BFM-2) says that ρ_A and ρ_B are compatible if and only if there exist decompositions of ρ_A and ρ_B

$$\begin{aligned} \rho_A &= p_0 |\chi\rangle\langle\chi| + \sum_{i>0} p_i |\psi_i\rangle\langle\psi_i| \\ \rho_B &= q_0 |\chi\rangle\langle\chi| + \sum_{j>0} q_j |\phi_j\rangle\langle\phi_j| \end{aligned}$$

which share a state $|\chi\rangle$ in common, such that $p_0, q_0 > 0$. (A given mixed density matrix can be written as an ensemble of pure states in many ways, the classification of the ensembles consistent with a given state can be seen in [Hughston *et al.* 1993] and [Nielsen 2000]).

BFM showed that in the case of finite dimensional systems both conditions are equivalent. However, it can be shown that in the case of infinite dimensional systems BFM-2 is in general invalid, whilst BFM-1 still makes sense as a criterion of compatibility [Herbut 2004].

Obviously one could choose compatibility criteria different from the ones stated above. For example, [Caves *et al.* 2002] study two different approaches to compatibility, one is based on the compatibility of *prior* beliefs and the second is based on the compatibility of *predictive* measurement probabilities. They show that the former is equivalent to BFM-1, whilst the latter leads to a hierarchy of measurement-based criteria inequivalent to BFM. Here we will concentrate on the BFM conditions (in fact our arguments will be based solely on BFM-1 compatibility), partly because of its simplicity for our objective, and also because it is consistent with the following desirable qualities:

1. If anyone describes a system by ρ , then nobody can find it in a pure state in the null space of ρ ;
2. A system that cannot be found to be in either of two distinct states cannot be found to be in any superposition of those states;
3. To be compatible the descriptions must represent a subset of a currently relevant body of information that could, in principle, all have been acquired by a single well-informed observer (i.e. it does not include the possibility of guesses in the state assignments of the observers).

In fact, an important consequence of the BFM criterion is that if *both* descriptions ρ_A and ρ_B are *pure* states, then they will only be compatible if they are identical:

$$\rho_A = \rho_B = \Psi.$$

This seems natural because pure states represent states of maximal knowledge (or minimal ignorance).

Now, armed with these tools let us study the question we are interested in, viz: When is a classical assignment compatible with a quantum one? (with classicality and quantumness defined as in section 1.5.1)

For the sake of simplicity let us concentrate on the case where Alice and Bob agree both on the Hilbert space \mathfrak{H} of the system and also on the partition $\{P_\mu\}$ w.r.t. which classicality is to be defined. If this is the case then it is obvious that if both ρ_A and ρ_B are *pure* and *compatible* then they must agree on whether the system belongs to $\tilde{C}_{\{P_\mu\}}$ or $\tilde{Q}_{\{P_\mu\}}$ (we will refer to this as the system being C or Q respectively). Therefore we will only study the case where at least one of the descriptions is mixed (not pure). Furthermore, without loss of generality we will assume that Alice's description is always mixed whilst Bob's state can be either mixed or pure.

If we analyse the case when $\dim \mathfrak{H} = 2$ and at least one of the descriptions, ρ_A or ρ_B , is a mixed state, then, according to BFM-1, ρ_A and ρ_B will *always* be compatible. This is easily seen since, if one of the states is mixed, say ρ_A , then its support will always coincide with the whole of \mathfrak{H} , and hence the intersection with $\text{supp}\{\rho_B\}$ will always be non-empty. Therefore, in the case of two-dimensional systems, for any state $\rho_B \in \tilde{Q}_{\{P_\mu\}}$ there will always exist a compatible mixed (non-extremal) state $\rho_A \in \tilde{C}_{\{P_\mu\}}$. That is, unless both observers give pure state assignments, then there will always be a potential ambiguity on whether the system is Q or C in spite of the assignments being compatible.

For $\dim \mathfrak{H} = 3$ there are very similar arguments. If ρ_A and ρ_B are both mixed states then they will always be compatible since there is not enough “space” in \mathfrak{H} to fit their supports without there being an intersection. If just one of the assignments is mixed, say ρ_A , with its support being a proper subset of \mathfrak{H} , then there exists a single/unique pure state that is incompatible with it. Namely the only case in which ρ_B can be incompatible with a mixed ρ_A is if $\dim \{\text{supp}\{\rho_A\}\} = 2$ and $\rho_B = |\psi_{A\perp}\rangle\langle\psi_{A\perp}|$, with $\rho_A |\psi_{A\perp}\rangle = 0$.

Now suppose that Alice describes the system by a mixed classical state $\rho_A \in \tilde{C}_{\{P_\mu\}}$, with $\dim \{\text{supp}\{\rho_A\}\} = 2$, and Bob assigns a mixed state, either Q or C. Then their states will always be compatible and we will have that there is the potential for an ambiguity on the Q-C question. If on the other hand Bob's state is pure and Q, i.e. $\rho_B \in \partial\tilde{Q}_{\{P_\mu\}}$, then it must be compatible with Alice's; whereas if Bob's pure state is to be incompatible with Alice's, then it will have to be an extremal classical state, i.e. $\rho_B \in \partial\tilde{C}_{\{P_\mu\}}$.

Alternatively, if Alice describes the system by a mixed quantum state $\rho_A \in \tilde{Q}_{\{P_\mu\}}$, $\dim \{\text{supp}\{\rho_A\}\} = 2$, the only case of interest that remains to be analyzed is if Bob assigns an extremal classical state $\rho_B \in \partial\tilde{C}_{\{P_\mu\}}$. In this scenario the question of compatibility depends on the particular states. However it is easy to convince one self that for any $\rho_A \in \tilde{Q}_{\{P_\mu\}}$ there exists at least one compatible $\rho_B \in \partial\tilde{C}_{\{P_\mu\}}$.

In summary, for $\dim \mathfrak{H} = 3$, we have that for any Q or C description of the state of the system there exists at least one BFM-1 compatible state with an opposing view on the Q-C question.

In general it is easy to see that if both ρ_A and ρ_B are mixed, and hence of rank $r_A \geq 2$ and $r_B \geq 2$ respectively ($\text{rank}\{\rho\} = \dim \{\text{supp}\{\rho\}\}$), then they will always be BFM-1 compatible

unless $\dim \{\mathfrak{H}\} \geq r_A + r_B$. However the question of the general classification of the compatibility of Q-C descriptions when $\dim \{\mathfrak{H}\} = N$, with $N \geq 4$, becomes very complicated. Nonetheless, we can obtain some definite answers if we concentrate on the question of whether, for a given classical description by Alice, there exists a compatible quantum description by Bob. The answer is obviously positive, i.e. for any mixed classical description there always exists a compatible mixed quantum description. The proof goes as follows:

If ρ_A is mixed and belongs to $\tilde{C}_{\{P_\mu\}}$, we have that

$$\rho_A = \sum_{k=1}^{r_A} \lambda_k^A P_k^A,$$

with $\forall k P_k^A \in \{P_\mu\}$, and by hypothesis $\lambda_k^A > 0$ and $2 \leq r_A \leq \dim \{\mathfrak{H}\}$. Then one can always construct a state

$$\rho_B = \sum_{k=1}^{M_B} p_k^B P_k^A + \Pi_Q^B$$

such that $2 \leq M_B \leq r_A$ and $\text{Tr} \left\{ \Pi_Q^B \right\} = 0$. Depending on the choice of Π_Q^B the state ρ_B can be either pure or mixed, but for ρ_B to satisfy the conditions defining a state, equations (1.8) to (1.10), Π_Q^B must always be such that:

$$\left(\sum_{k=1}^{M_B} P_k^A \right) \Pi_Q^B = \Pi_Q^B.$$

Thus the support of ρ_B is contained *a fortiori* in the span of $\{P_k^A\}_{k=1}^{M_B}$ which in turn implies

$$\text{supp} \{\rho_B\} \subseteq \text{supp} \{\rho_A\},$$

which proves that for any mixed classical state one can construct a BFM-1 compatible, mixed or pure, quantum state.

In conclusion we have shown that, as expected, there is ample room for ambiguity when two observers try to decide whether a particular system belongs to $\tilde{C}_{\{P_\mu\}}$ or $\tilde{Q}_{\{P_\mu\}}$. The only case where there seems to be absolutely no uncertainty is when they have previously agreed on the partition $\{P_\mu\}$ w.r.t. which they define classicality, and if both of the observers assign a pure state to the system. The study of the case of where Alice and Bob consider different partitions of \mathfrak{H} to define classicality remains as future work.

This possibility of disagreement between observers on whether a given system is classical or quantum points to the generally accepted view that the boundary between quantum and classical behaviour is not clear cut, and thus questions the “general” validity of our classicality criterion and of the crisp splitting of the state space into two (static) sets \tilde{C} and \tilde{Q} . In fact, this problem arising from possible disagreements is only compounded by the fact that even the choice of the partition, with respect to which both Alice and Bob have agreed to describe classicality, is in itself a context dependent property. However, as mentioned in section 1.5.1 this is not necessarily a bad thing. At least it shows that our criteria for classicality and quantumness are consistent with some of the ingredients of the Copenhagen interpretation.

In spite of these difficulties, we will continue to use these criteria for quantumness and classicality because: for one, they coincide with the ones used in the vast majority of decoherence studies [Giulini *et al.* 1996] [Zurek 2003], and therefore will allow us to compare our results with the ones in the existing literature; and two, it provides us with a working tool to study the C-Q transition that is consistent with the Copenhagen interpretation (it does not solve the context dependency a lot of authors would like to get rid of, but it gives us a criterion to study the transition within the limitations of the Copenhagen interpretation).

Chapter 3

Review of Open System Dynamics

Throughout the rest of the thesis we will be constantly making use of the dynamics of open systems, that is, systems interacting with an unobservable environment and whose dynamics differ from the usual Schrödinger equation. Therefore, so as to introduce the tools we will be using, we will review what are the usual methods used for the descriptions of such systems.

The general philosophy we will use to deal with open systems is to suppose that one is able to identify a “relevant” subset of degrees of freedom of the total system, the universe of discourse, that is accessible to experimental observations and manipulation (or that are principally responsible for the behaviour we are trying to model). We will call this the *system of interest* or relevant system, and whenever necessary denote it by S (in general it will be evident from the context whether S refers to the system of interest or to the state space of the system of interest, nonetheless, to avoid confusion when referring to the state space we will always write $S(\mathfrak{A})$). The rest of the universe we will call the *environment* and denote it by E . Furthermore we will suppose that we can extend our choice of the environment in such a manner that the dynamics of the total system, S plus E , can be approximated by the usual unitary evolution of conventional (non-relativistic) Quantum Mechanics. In other words, we will assume that the dynamics of the total system can be described by a unitary evolution operator which obeys the Schrödinger equation. However, except for some very simple cases, it is impractical (and even sometimes apparently impossible) to solve this equation for the total system $S \cup E$, hence the introduction of the tools of this chapter.

For completeness, we will include some of the most commonly used methods although we will not use all of them. This is especially the case of sections 3.1 and 3.6 where we briefly mention some tools that are regularly employed but, due to practical reasons, will not be explicitly used in the rest of this thesis.

3.1 Master equations (constructive approach)

Following our previous comments, let us suppose that the system of interest, S , is coupled to an environment E (for example a reservoir or heat bath), and that the total system, $S \cup E$, is closed. In this case the dynamics of the state of the total system are dictated by the von Neumann equation generated by a Hamiltonian of the form:

$$H_{S \cup E} = H_S \otimes 1_E + 1_S \otimes H_E + gV_{SE}, \quad (3.1)$$

where H_x represents the Hamiltonian that the system x would obey if it were closed, g is a coupling constant that will be used to keep track of approximations, and V_{SE} represents the interaction between the system of interest and the environment. Under these assumptions the dynamics of the state of S , $\rho = \text{Tr}_E \{\rho_T\}$ (where ρ_T is the density matrix of the total system $S \cup E$), would be given by

$$\frac{d}{dt}\rho(t) = \text{Tr}_E \{[H_{S \cup E}, \rho_T(t)]\}.$$

However this equation depends on the state of the total system at time t , thus what we would ideally like to have is an equation solely dependent on $\rho(t)$, i.e. a *master equation* for S .

An ingenious method (consistent with the assumptions stated above) first introduced by [Nakajima 1958] and [Zwanzig 1960] allows one to obtain a master equation for ρ , the state of the principal system. The main idea behind the Nakajima-Zwanzig method is to use a projector (superoperator) to project the state of the total system onto that of the relevant system. The choice of the projector to be used depends on the problem to be studied, and ultimately on what we consider to be the system of interest. For example, if the relevant system only involves populations, and not the coherent terms, one could choose to project onto the diagonal elements of ρ in some suitable basis thus obtaining a “classical” Pauli master equation [Fain 2000]. However, this is a very particular case and in general we are interested in determining ρ . A typical choice for this purpose is to define the projector as $\hat{P}\rho_T = \text{Tr}_E \{\rho_T\} \otimes \omega_E^{(ref)} = \rho \otimes \omega_E^{(ref)}$, where the choice of the reference state of the environment, $\omega_E^{(ref)}$, is fixed by the physical context. For this projector the method gives rise to an exact master equation of the form (for a detailed derivation and for techniques to construct projectors see [Fick & Sauermann 1990]):

$$\frac{d}{dt}\rho(t) = -\frac{i}{\hbar} \left[H_S + \langle gV_{SE} \rangle_{\omega_E^{(ref)}}, \rho(t) \right] + \int_{t_0}^t \hat{K}(t-\tau) \rho(\tau) d\tau + \hat{R}(t) \rho_T(t_0). \quad (3.2)$$

This equation is usually called a *generalized master equation*, or Nakajima-Zwanzig equation. The kernel of the convolution, which accounts for the residual interaction of S with the environment, is given by:

$$K(t-\tau) \rho(\tau) = \text{Tr}_E \left\{ \hat{\mathcal{L}}_{SE} \hat{Q} e^{\hat{\mathcal{Q}} \hat{\mathcal{L}}_{SE} \hat{Q}(t-\tau)} \hat{Q} \hat{\mathcal{L}}_{SE} \left[\rho(\tau) \otimes \omega_E^{(ref)} \right] \right\},$$

where $\hat{\mathcal{L}}_{SE}$ is the Liouvillian superoperator of the total system, $\hat{\mathcal{L}}_{SE} \bullet = -\frac{i}{\hbar} [H_{S \cup E}, \bullet]$, and \hat{Q} is the complement of \hat{P} , $\hat{Q} = \hat{\mathbf{1}} - \hat{P}$. The inhomogeneous term, responsible for propagating correlations which exist in the “irrelevant” part of the initial state of the total system, is given by

$$\hat{R}(t) \rho_T(t_0) = \text{Tr}_E \left\{ \hat{\mathcal{L}}_{SE} \hat{Q} e^{\hat{\mathcal{Q}} \hat{\mathcal{L}}_{SE} \hat{Q} t} \rho_T(t_0) \right\}.$$

Unfortunately the integro-differential equation (3.2) is usually as difficult to solve as the von Neumann equation for the total system (for a few solvable examples and illustrations of the difficulties see [Haake 1973]). These difficulties are not only related to solving a set of coupled integro-differential equations, even the determination of the convolution kernel can be quite a daunting task. In fact, there is a similar procedure using projection superoperators that, in certain cases, can be used to obtain a “time-convolutionless” master equation yielding an ordinary differential equation [Chaturvedi & Shibata 1979]; but in this case as well the determination of

the terms involved in the master equation is, in general, only achievable if one uses some sort of perturbation expansion [Breuer & Petruccione 2002].

Let us mention some of the most typical simplifications used in the literature that can be performed under certain assumptions [van Wonderen & Lendi 1995] [Breuer & Petruccione 2002]. The most common one is to assume that the total system has as an initial condition an uncorrelated state, i.e. $\rho_T(t_0) = \rho(t_0) \otimes \rho_E(t_0)$. Then the inhomogeneous term (the third on the rhs of 3.2) goes to zero. Another one is the so-called Born approximation which is valid for weak couplings and involves truncating the interaction terms up to second order in the interaction coupling g (this is used for calculating the kernel). Another is the Markov approximation which supposes that the environment possesses no memory (a very short correlation time or an infinite recurrence time). This allows us to extend the limits of integration of the convolution to the entire interval $t \in [0, \infty)$. The problem with these approximations is that they do not preserve the positivity condition (1.10) for all initial conditions (concrete examples of this violation can be seen in [Suarez *et al.* 1992], however one can circumvent this problem by limiting the domain of definition of the master equation to a set that yields positive solutions [Benatti *et al.* 2003], further conditions for positivity can be found in [Wilkie 2000]). Actually, the problem of preserving positivity is a recurring theme that we will encounter repeatedly in most of this thesis.

It is perhaps worth mentioning that if one is to use the previous approximations it is easier to start directly from the von Neumann equation with the uncorrelated initial condition, then use a second order (Born approximation) Dyson expansion of the unitary propagator, and if physically justified then use the Markov limit to obtain a time-local master equation. A detailed description of these steps and an expression of the resulting master equation can be seen in [Paz & Zurek 2000]. For a detailed analysis of the physical validity of the approximations used in this setting we refer the reader to [Alicki 2002].

3.2 Generalized maps

Given the difficulties of obtaining, and working with, master equations mentioned in the previous section we will explore a more axiomatic approach for the description of open systems.

The time evolution of the state describing our system is given in the most general case by a mapping, or superoperator, $\hat{\Lambda}$ with domain $\text{dom} \left\{ \hat{\Lambda} \right\} \cap S(\mathfrak{A}) \neq \emptyset$, and $\text{range} \left\{ \hat{\Lambda} \right\} \cap S(\mathfrak{A}) \neq \emptyset$ (for reasons that will become apparent in future sections we will need to consider dynamical maps that are not endomorphisms for the whole of $S(\mathfrak{A})$), such that:

$$\rho(t) = \hat{\Lambda}_{t,t_0,\vec{\kappa}}[\rho(t_0)]. \quad (3.3)$$

Here $\vec{\kappa}$ represents a discrete set of parameters characterizing the dynamics of the system. However, if the map $\hat{\Lambda}$ is to transform states into states then it must obey some basic requirements, namely it should preserve the conditions (1.8) to (1.10) that characterize a density matrix (Hermiticity, positivity, and normalization) at least for some subset of states belonging to $\text{dom} \left\{ \hat{\Lambda} \right\}$.

To analyse the type of conditions on $\hat{\Lambda}$ that result from preserving these properties let us restrict ourselves to systems of finite dimension N , and to maps that are defined and *linear* over the whole of $\mathfrak{B}(\mathfrak{H}) (\supseteq S(\mathfrak{A}))$. Then, using the operator sum expansion described in appendix A,

for an arbitrary basis $\{B_\mu\}_{\mu=0}^{N^2-1}$ the condition of preserving Hermeticity implies¹

$$\hat{\Lambda}_{\mu\nu} \mathfrak{X}_{\nu\alpha} = \mathfrak{X}_{\mu\nu} \overline{\hat{\Lambda}_{\nu\alpha}}, \quad (3.4)$$

where the components of the superoperator are given by

$$\hat{\Lambda}_{\mu\nu} = \left\langle \left\langle B_\mu \left| \hat{\Lambda} \right| B_\nu \right\rangle \right\rangle = \text{Tr} \left\{ B_\mu^\dagger \left(\hat{\Lambda} [B_\nu] \right) \right\}, \quad (3.5)$$

and the elements of the symmetric matrix \mathfrak{X} are

$$\mathfrak{X}_{\mu\nu} := \text{Tr} \left\{ B_\mu^\dagger B_\nu^\dagger \right\}. \quad (3.6)$$

The conservation of trace requires that

$$\hat{\Lambda}_{\mu\nu} \text{Tr} \left\{ B_\mu^\dagger \right\} = \text{Tr} \left\{ B_\nu^\dagger \right\}. \quad (3.7)$$

The conditions on $\hat{\Lambda}$ for it to preserve the positive semidefinite character of the spectrum of ρ will be addressed in future sections.

In the particular case where we describe the system using a canonical basis $B_{\mu=[ij]} = |i\rangle \langle j|$, we have that $\mathfrak{X}_{kl,ij} = \delta_{il} \delta_{jk}$. This means that (3.4) turns into $\hat{\Lambda}_{nm,ij} = \overline{\hat{\Lambda}_{mn,ji}}$, and condition (3.7) becomes $\sum_n \hat{\Lambda}_{nn,qr} = \delta_{qr}$.

If the basis is formed by a set of Hermitian operators (e.g. the generators of $\text{SU}(N)$) then we would have $\mathfrak{X}_{\mu\nu} = N \delta_{\mu\nu}$, then (3.4) reads as $\hat{\Lambda}_{\mu\nu} = \overline{\hat{\Lambda}_{\nu\mu}}$. If besides Hermeticity of the basis we also have that $B_0 = \mathbf{1}$ then the trace condition would be $\hat{\Lambda}_{00} = 1$ and $\hat{\Lambda}_{0i} = 0$. For such a basis the map could be represented as:

$$\hat{\Lambda}_{t,\vec{\kappa}} = \begin{pmatrix} 1 & \vec{0} \\ \vec{f}(t, \vec{\kappa}) & \mathbb{A}(t, \vec{\kappa}) \end{pmatrix} \quad (3.8)$$

where: 1 is a scalar, $\vec{0}$ is a $N^2 - 1$ row vector with all its entries equal to zero, $\vec{f}(t, \vec{\kappa})$ is a $N^2 - 1$ column vector, and $\mathbb{A}(t, \vec{\kappa})$ is a $(N^2 - 1) \times (N^2 - 1)$ matrix. If $\hat{\Lambda}$ possesses a unique fixed point then this state will in general coincide with $\rho \sim \left(1, \vec{f}(t, \vec{\kappa}) \right)^T$. See for example equation (5.37) in section 5.6.

The previous has considered the dynamics of the state $\rho(t)$, i.e. the equivalent of the Schrödinger picture. However, if all the information about the system is obtained via quantities like $\text{Tr} \{ \rho(t) A \}$, then, at least in principle, we could fix the state and only consider the dynamics of the observables. The corresponding Heisenberg picture evolution is defined through the duality

$$\text{Tr} \left\{ \hat{\Lambda}_{t,t_0,\vec{\kappa}} [\rho(t_0)] A(t_0) \right\} = \text{Tr} \left\{ \rho(t_0) \hat{\Lambda}_{t,t_0,\vec{\kappa}}^* [A(t_0)] \right\} \quad (3.9)$$

¹It is worth pointing out that our condition (3.4) differs from the one stated in [Sudarshan & Shaji 2002]. However, in a personal communication the authors of the cited article have admitted that their condition is incorrect.

Observe that if $\hat{\Lambda}$ is trace preserving then its dual must obey $\hat{\Lambda}_{t,\vec{\kappa}}^*[\mathbf{1}] = \mathbf{1}$ ($\text{Tr} \left\{ \mathbf{1} \hat{\Lambda}_{t,\vec{\kappa}}[\rho(t_0)] \right\} = \text{Tr} \left\{ \hat{\Lambda}_{t,\vec{\kappa}}^*[\mathbf{1}] \rho(t_0) \right\} = \text{Tr} \left\{ \mathbf{1} \rho(t_0) \right\} = \text{Tr} \left\{ \rho(t_0) \right\}$). Dual maps that obey this property will be called unital. For finite systems and an arbitrary basis the dual is simply the Hermitian conjugate, viz.

$$\hat{\Lambda}_{\mu\nu}^* = \overline{\hat{\Lambda}_{\nu\mu}} \quad (3.10)$$

Nonetheless it is important to observe that whenever there is dissipation one needs to be careful when working in the Heisenberg picture since the maps $\hat{\Lambda}_t^*$ are not in general automorphisms of the algebra \mathfrak{A} . That is, in the case of open systems we will generally have that (see equation 3.22)

$$\hat{\Lambda}_t^*[AC] \neq \left(\hat{\Lambda}_t^*[A] \right) \left(\hat{\Lambda}_t^*[C] \right).$$

Therefore when calculating the expectation value of an observable we will use the definition of the operator at time zero so as to satisfy the relation (3.9). However, we will still be interested in quantities like $\left(\hat{\Lambda}_t^*[A] \right) \left(\hat{\Lambda}_t^*[C] \right)$, since we can use them to construct what would be the effective algebra associated with the system of interest at time t .

3.3 Completely positive maps

Now we would like to start addressing the issue that for $\hat{\Lambda}$ to be physically valid (or consistent with a statistical interpretation of ρ) it needs to preserve the positivity of ρ , i.e.

$$\text{Tr} \left\{ A^\dagger A \hat{\Lambda}[\rho] \right\} \geq 0 \quad \forall A \in \mathfrak{B}(\mathfrak{H}). \quad (3.11)$$

A map $\hat{\Lambda}$ that satisfies this property, for every ρ , will be called a positive map. For now we will assume that this condition needs to be valid for every initial state ρ , in future sections we will relax this condition.

A typical argument regarding positivity goes as follows: If we consider that in principle it is always possible to extend the system of interest such that it includes another system, w , with Hilbert space, \mathfrak{H}_w , of dimension N_w and trivial isolated dynamics $H_w = 0$, placed sufficiently far away from the original system of interest such that there is no interaction. Then one could argue that for the map $\hat{\Lambda}$ to be physically realizable then $\hat{\Lambda} \otimes \hat{\mathbf{1}}_{N_w}$ should also be positive ($\hat{\mathbf{1}}_{N_w}$ is the identity superoperator acting on $\mathfrak{B}(\mathfrak{H}_w)$). If the transformation $\hat{\Lambda} \otimes \hat{\mathbf{1}}_{N_w}$ is positive for any $N_w = 1, 2, \dots$ then the map is said to be *completely positive*.

Completely positive maps on operator algebras were studied already in the 50's, and the celebrated Stinespring representation [Stinespring 1955] leads to a general form of completely positive map often called Kraus decomposition [Kraus 1983]:

$$\hat{\Lambda}\rho_0 = \sum_{\eta} W_{\eta} \rho_0 W_{\eta}^{\dagger}, \quad (3.12)$$

where $W_{\eta} \in \mathfrak{B}(\mathfrak{H})$ (obviously $\rho_0 \in \mathfrak{B}(\mathfrak{H})$). It is evident that this type of map preserves Hermiticity, but if the map is to be trace preserving as well then the ‘‘Kraus’’ operators need to satisfy

$$\sum_{\eta} W_{\eta}^{\dagger} W_{\eta} = \mathbf{1}. \quad (3.13)$$

The decomposition (3.12) is highly non-unique, in particular the sum over η can be replaced by an integral. As well, if the system of interest is of finite dimension N then one can always find a Kraus decomposition with at most N^2 distinct terms[Alicki 2002].

From the definition of the dual map in (3.9) it is easy to see that for a completely positive map the Heisenberg picture dynamics are given by

$$\hat{\Lambda}^* A = \sum_{\eta} W_{\eta}^{\dagger} A W_{\eta} \quad \forall A \in \mathfrak{B}(\mathfrak{H}). \quad (3.14)$$

If we define the linear superoperators

$$\hat{L}_A B := AB, \quad (3.15)$$

and

$$\hat{R}_A B := BA, \quad (3.16)$$

(with $A, B \in \mathfrak{B}(\mathfrak{H})$)² then we can conveniently write a completely positive map as

$$\hat{\Lambda} = \sum_{\eta} \hat{L}_{W_{\eta}} \hat{R}_{W_{\eta}^{\dagger}}. \quad (3.17)$$

The symbolic form of the Kraus operators for a dynamic map is relatively easy to obtain. If we suppose *uncorrelated initial conditions*, and that the final time t is fixed, then we have

$$\rho(t) = \text{Tr}_E \left\{ U_t (\rho(0) \otimes \omega_E(0)) U_t^{\dagger} \right\}, \quad (3.18)$$

with $U_t = \exp \left\{ -\frac{i}{\hbar} H_{S \cup E} t \right\}$. Then, by using the spectral decomposition $\omega_E(0) = \sum_{\alpha=1}^{N_E} \lambda_{\alpha} |\lambda_{\alpha}\rangle \langle \lambda_{\alpha}|$, we can write

$$\rho(t) = \sum_{\alpha, \beta=1}^{N_E} W_{\alpha\beta}(t) \rho(0) W_{\alpha\beta}^{\dagger}(t), \quad (3.19)$$

where, if $\{|n\rangle\}_{n=1}^N$ is a complete orthonormal basis for \mathfrak{H} , the Kraus operators are given by

$$\langle m | W_{\alpha\beta}(t) | n \rangle = \sqrt{\lambda_{\beta}} \langle m, \lambda_{\alpha} | U_t | n, \lambda_{\beta} \rangle \quad (3.20)$$

(in equation 3.12 we have implicitly collected the indices as $\eta = [\alpha\beta]$).

It is important to emphasise that the previous analysis supposes an uncorrelated initial state, and that there exists a debate in the literature on whether every physical map is completely positive, especially when there exist initial correlations between the system of interest and the environment in the initial state of the total system. We will address these issues in section 3.5.

²Some useful properties obeyed by these superoperators are: $[\hat{L}_A, \hat{R}_B] = 0$, $\hat{L}_A \hat{L}_B = \hat{L}_{AB}$, and $\hat{R}_A \hat{R}_B = \hat{R}_{BA}$ $\forall A, B \in \mathfrak{B}(\mathfrak{H})$.

3.4 Markovian and completely positive dynamics

In the previous section we introduced a dynamical map $\hat{\Lambda}_t$, generated by the Kraus operators in (3.20), which if we allow t to vary would give a one-parameter family $\{\hat{\Lambda}_t\}_{t \geq 0}$ of dynamical maps ($\hat{\Lambda}_{t=0} = \hat{\mathbf{1}}$). Such a family describes the whole future time evolution of the system of interest, which, in general, could be very involved. However, if the characteristic time-scales over which the environment correlation functions decay are much smaller than the characteristic time-scale of the isolated evolution of the system of interest, one could argue that it is justifiable to neglect memory effects. As in the classical theory one thus expects Markovian-type behaviour and hence time-local dynamics. This can be formalized by requiring that the family of dynamical maps obeys the *semigroup* composition property

$$\hat{\Lambda}_t \hat{\Lambda}_s = \hat{\Lambda}_{t+s} \quad \forall t, s \geq 0,$$

and that $\text{Tr} \{A \hat{\Lambda}_t [\rho(0)]\}$ is a continuous function of t for any $A \in \mathfrak{B}(\mathfrak{H})$. (These conditions are in addition to the basic requirements of preserving trace, Hermiticity, and positivity).

Then it can be proved [Gorini *et al.* 1976][Lindblad 1976] that there exists a linear map \hat{D} , called the generator of the semigroup, such that

$$\frac{d}{dt} \rho(t) = \hat{D} [\rho(t)],$$

where $\rho(t) = \hat{\Lambda}_t \rho(0)$. We will call this type of dynamics Markovian.

Notice that we could have just as easily written the Markovian equation as

$$\frac{d}{dt} \hat{\Lambda}_t = \hat{D} \hat{\Lambda}_t \quad \forall t \geq 0.$$

The generator \hat{D} satisfies the *dissipative* condition (Kadison inequality) [Bratelli & Robinson 1987]³:

$$\hat{D}^* [A^\dagger B] \geq \hat{D}^* [A^\dagger] B + A^\dagger \hat{D}^* [B] \quad \forall A, B \in \mathfrak{B}(\mathfrak{H}), \quad (3.21)$$

with equality only achieved if the map is *reversible*. (It is easy to see that equality is trivially satisfied in the blatantly reversible case of unitary dynamics obeying the von Neumann equation, where we would have $\hat{D}_{vN}^\bullet = \frac{i}{\hbar} [H, \bullet]$ and the maps would actually form a one-parameter group over time). If the map is trace preserving then we have that the Heisenberg picture evolution satisfies [Bratelli & Robinson 1987]:

$$\hat{\Lambda}_t^* [AB] \geq \hat{\Lambda}_t^* [A] \hat{\Lambda}_t^* [B], \quad (3.22)$$

where again equality only occurs when $\hat{\Lambda}_t^*$ is a reversible automorphism.

It can be shown that in this Markovian limit, for completely positive dynamics, the generator of the semigroup can always be written as:

$$\hat{D} \rho(t) = -\frac{i}{\hbar} [H, \rho(t)] + \frac{1}{2} \sum_{\alpha} \left\{ [V_{\alpha} \rho(t), V_{\alpha}^\dagger] + [V_{\alpha}, \rho(t) V_{\alpha}^\dagger] \right\}. \quad (3.23)$$

³Following the usual convention in the literature, whenever we write $A \geq B$, with $A, B \in \mathfrak{B}(\mathfrak{H})$, we mean that $(A - B)$ is a positive operator.

[Gorini *et al.* 1976] have shown that this is the most general generator of a Markovian dynamical map in the case of a finite dimensional Hilbert space of the system of interest. Independently [Lindblad 1976] proved that (3.23) is the most general form of a *bounded* generator for any separable Hilbert space if one admits countable sets of indices $\{\alpha\}$. Equation (3.23) is usually referred to as the Lindblad equation.

If we use the left and right superoperators introduced in (3.15) and (3.16), and the Liouvillian $\hat{\mathcal{L}}_H = \hat{L}_H - \hat{R}_H$, then we can rewrite the generator (3.23) as

$$\hat{D} = -\frac{i}{\hbar}\hat{\mathcal{L}}_H + \sum_{\alpha} \left\{ \hat{L}_{V_{\alpha}} \hat{R}_{V_{\alpha}^{\dagger}} - \frac{1}{2} \hat{R}_{V_{\alpha}} \hat{R}_{V_{\alpha}^{\dagger}} - \frac{1}{2} \hat{L}_{V_{\alpha}^{\dagger}} \hat{L}_{V_{\alpha}} \right\}. \quad (3.24)$$

The first term of the generator, $\frac{i}{\hbar}\hat{\mathcal{L}}_H$, represents the unitary part of the dynamics generated by the Hamiltonian H . However this Hamiltonian does not coincide in general with the bare Hamiltonian of the system of interest, the coupling with the environment usually results in a “Lamb shift” as exemplified in (3.2). We will refer to the operators V_{α} as Lindblad operators, and to the term in brackets as the dissipative component of the generator.

The problem with the Lindblad equation is that there is no universally valid recipe to determine the dissipative component from first principles, this usually has to be done phenomenologically. Nonetheless, since the Lindblad equation is the most general form (for a completely positive semigroup) it turns out that all known Markovian master equations, with uncorrelated initial conditions, can be manipulated to have this form. For some examples of master equations in the Markovian and weak-coupling (Born) limit one can consult [Gardiner & Zoller 2000]. Yet, we must emphasize that the approach leading to the Lindblad equation does not employ any explicit assumptions about the strength of the interaction between the system of interest and the environment; it only assumes the semigroup property. But, as we will see in the next section, the semigroup, or Markovian, character seems to be related to the strength of the coupling and the initial condition of the state of the total system. For some approximation methods for constructing Lindblad equations see [Alicki & Lendi 1987] and [Lidar *et al.* 2001]; also [Kosloff *et al.* 1997] has a presentation of some of the most important/common choices for Lindblad operators occurring in physical systems.

Finally, we remark that the generator \hat{D} does not uniquely fix the form of the Hamiltonian H and the Lindblad operators V_{α} . In fact, the generator is invariant under the following transformations:

- Unitary transformations of the set of Lindblad operators,

$$V_{\alpha} \rightarrow V'_{\alpha} = \sum_{\beta} u_{\alpha\beta} V_{\beta},$$

where $u_{\alpha\beta}$ is a unitary matrix;

- Inhomogeneous transformations

$$\begin{aligned} V_{\alpha} &\rightarrow V'_{\alpha} = V_{\alpha} + a_{\alpha} \mathbf{1}, \\ H &\rightarrow H' = H + \frac{1}{2i} \sum_{\alpha} \left\{ \overline{a_{\alpha}} V_{\alpha} - a_{\alpha} V_{\alpha}^{\dagger} \right\} + b \mathbf{1}, \end{aligned}$$

where $\{a_{\alpha}\}$ are complex scalars and b is real.

3.5 Initial correlations, positivity, and general maps

In the previous two sections we have assumed that the dynamical map $\hat{\Lambda}_t$ is completely positive (this choice of dynamics is usually taken for granted in the vast majority of the quantum information literature). Nonetheless, there has been some debate regarding this assumption [Alicki 1995] [Pechukas 1995]. Complete positivity results in some very strict restrictions on the dynamics the system can obey. In particular it imposes non-trivial constraints on the relaxation rates of the system of interest [Schirmer & Solomon 2004]. For example, in the case of a two-level system, complete-positivity implies that the off-diagonal relaxation time, τ_\perp , is related to the diagonal relaxation time, τ_\parallel , by the usual Bloch relation $\tau_\perp \leq 2\tau_\parallel$, as is in fact usually observed in experiments in various fields, e.g. nuclear magnetic resonance [Cowan 1997] and quantum optics [Allen & Eberly 1987]. (For an example of a completely positive map satisfying this Bloch relation see section 5.6). However, some numerical simulations of strongly interacting systems indicate that the exponential decay may not always conform to this rule [Chang & Skinner 1993] (see also [Laird *et al.* 1994]). This caused some surprise, prompting [Pechukas 1994] to doubt the argument for complete positivity in section 3.3, specifically he noted that: “It is very powerful magic: w sits apart from $S \cup E$ and does nothing; by doing so, it forces the motion of S to be completely positive, with dramatic consequences such as $\tau_\perp \leq 2\tau_\parallel$.” He went on to argue that complete positivity is an artifact of uncorrelated initial conditions (between S and E), and that, in general, dynamics need not be completely positive. This has been confirmed by several other authors, e.g. [Royer 1996] and [Stelmachovic & Buzek 2001]. Some explicit examples of non-completely-positive dynamical maps resulting from the existence of initial correlations between the system of interest and the environment can be seen in [van Wonderen & Lendi 2000], [Fonseca-Romero *et al.* 2004] and [Jordan *et al.* 2004]. In particular van Wonderen and Lendi show that, for their example, the Bloch relation does not hold when the initial state is entangled.

Since in future chapters we will be interested in the structure of some of these non-completely-positive maps, let us study further their structure, for this we will follow some of the arguments in [Stelmachovic & Buzek 2001]. Their arguments run more or less as follows. Suppose that both the system of interest and the environment are of finite dimensions, N_S and N_E respectively. Then, using the techniques in appendix A, expand the state of the composite system in the basis $\{B_m^S \otimes B_\mu^E\}$, with $m = 0, \dots, (N_S^2 - 1)$, and $\mu = 0, \dots, (N_E^2 - 1)$, and where $B_m^\bullet \in \mathfrak{B}(\mathfrak{H}_\bullet)$. Furthermore choose the basis such that $B_m^S \otimes B_\mu^E$ is Hermitian, and $B_0^S \otimes B_0^E = \mathbf{1}_S \otimes \mathbf{1}_E = \mathbf{1}_T$ (for example we could use the tensor product of the generators of $SU(N_S)$ and $SU(N_E)$ to construct this basis). Then the state of the total system can be written as

$$\rho_T = \frac{1}{N_S N_E} (\mathbf{1}_T + a_i B_i^S \otimes \mathbf{1}_E + b_\nu \mathbf{1}_S \otimes B_\nu^E + c_{i\nu} B_i^S \otimes B_\nu^E),$$

where, as usual, we have used the Einstein summation convention and $i = 1, \dots, (N_S^2 - 1)$; $\nu = 1, \dots, (N_E^2 - 1)$.

By using $\rho_S = \text{Tr}_E \{\rho_T\}$, $\rho_E = \text{Tr}_S \{\rho_T\}$, and some trivial algebra we can rewrite an arbitrary state of the total system as:

$$\rho_T = \rho_S \otimes \rho_E + \frac{1}{N_S N_E} (c_{i\nu} - a_i b_\nu) B_i^S \otimes B_\nu^E.$$

To simplify the notation let us define a new parameter

$$\gamma_{i\nu} := \frac{1}{N_S N_E} (c_{i\nu} - a_i b_\nu),$$

which is a measure of the correlation between S and E in ρ_T , and is explicitly given by

$$\gamma_{i\nu} = \frac{1}{N_S N_E} (\text{Tr}_T \{ (B_i^S \otimes B_\nu^E) \rho_T \} - \text{Tr}_S \{ B_i^S \rho_S \} \text{Tr}_E \{ B_\nu^E \rho_E \}). \quad (3.25)$$

Thus, if U_t is the time evolution operator for the total system, we have

$$\rho_S(t) = \text{Tr}_E \left\{ U_t (\rho_S \otimes \rho_E) U_t^\dagger \right\} + \gamma_{i\nu} \text{Tr}_E \left\{ U_t (B_i^S \otimes B_\nu^E) U_t^\dagger \right\},$$

which, given the arguments leading to equation (3.19), can always be written as

$$\rho_S(t) = \sum_{\alpha, \beta=1}^{N_E} W_{\alpha\beta}(t) \rho_S W_{\alpha\beta}^\dagger(t) + \gamma_{i\nu} \text{Tr}_E \left\{ U_t (B_i^S \otimes B_\nu^E) U_t^\dagger \right\}. \quad (3.26)$$

This is the expression we were after; we see that the evolution of S in the case of initial correlations consists of two terms. The first term corresponds to the standard Kraus representation of completely positive dynamics resulting from an uncorrelated initial state. The second term on the rhs of (3.26), for a fixed Hamiltonian of the total system, depends *solely* on the correlation parameters $\gamma_{i\nu}$ that do not explicitly depend on the choice of the initial state of the system of interest S (see below). In other words, these parameters cannot be determined by performing a local measurement on the initial state of S .

However, notice that the arguments in [Stelmachovic & Buzek 2001] are unduly complicated and restrictive. Their algebra, used above, only obscures the fact that they have written the state of the total system as

$$\rho_T = \rho_S \otimes \rho_E + (\rho_T - \rho_S \otimes \rho_E),$$

which is a valid expression independent of the dimensionality of the system of interest and of the environment. Nonetheless, the reduced dynamics of the system of interest can still be written in the form:

$$\rho_S(t) = \hat{\Lambda}_t^{Kraus} [\rho_S(0)] + \text{Tr}_E \left\{ U_t (\rho_T - \rho_S \otimes \rho_E) U_t^\dagger \right\}, \quad (3.27)$$

which does not necessarily correspond to a completely positive map.

Before continuing, let us make the trivial observation that if there is no effective coupling and therefore $U_t = U_t^S \otimes U_t^E$ then the inhomogeneous term disappears (the second one on the rhs of 3.27). Also, [Hayashi *et al.* 2003] proved that the inhomogeneity cancels if the total state and the coupling satisfy

$$\text{Tr}_E \{ V_{SE} (\rho_T - \rho_S \otimes \rho_E) \} = 0,$$

where V_{SE} is the interaction term of the Hamiltonian (see equation 3.1).

The question of what are the possible states ρ_T of the total system that result in a given ρ_S , i.e. a “blow-up” map $\Phi : \rho_S \rightarrow \rho_T$ such that $\rho_S = \text{Tr}_E \{ \rho_T \}$, has been studied by [Pechukas 1994], [Stelmachovic & Buzek 2001], [Fonseca-Romero *et al.* 2004], and [Jordan *et al.* 2004]. Although

they consider different examples their main results agree, and they can be summarized as a generalization of a theorem by Pechukas, that in the version of Fonseca-Romero *et al.* reads:

The state $\rho_T = \Phi\rho_S$ must be factorizing, $\rho_T = \rho_S \otimes \rho_E$, if the following conditions are to be satisfied:

1. The corresponding blow-up map of the preparation is a linear map in the sense that it preserves convex mixtures;
2. ρ_T is a proper state for $S \cup E$, i.e. it is positive;
3. Two different complete sets of pure states can be prepared in the considered preparation class.

It is worthwhile pointing out that this last condition cannot always be fulfilled. In particular Fonseca-Romero *et al.* consider an example where the total system, formed by two qubits, is in thermal equilibrium and in which one can only prepare a unique complete orthonormal set of state vectors for the system of interest; thus violating the third condition. In fact, it is well known that if ρ_T is a Gibbs state then, in general, it will only be factorizable in the case of *weak coupling* between S and E [Spohn 1980].

The point is that the generally accepted scheme for reduced dynamics is to say that the dynamical map is given by:

$$\rho_S \mapsto \hat{\Lambda}_t \rho_S = \text{Tr}_E \left\{ U_t (\Phi \rho_S) U_t^\dagger \right\}.$$

But if we require that the three previous conditions are satisfied then we will restrict ourselves to the uncorrelated case, which beyond the weak coupling regime is inappropriate. Therefore, we need to sacrifice one of the three conditions. For example, Pechukas proposal is to give up the positivity requirement for every state. This means, that we need to restrict ourselves to states ρ_S such that $\Phi \rho_S \geq 0$. This restriction to a subset of the possible states of S will be a recurring theme in various parts of this thesis. The nonlinear option has been explored by [van Wonderen & Lendi 2000] and [Fonseca-Romero *et al.* 2004]. They find that the nonlinear map is not uniquely defined for a given ρ_S .

Now let us return to equation (3.26), and in analogy with it let us define the affine map, \hat{M} , which $\forall \rho_S(0) \in S(\mathfrak{A})$ is given by

$$\hat{M}_t[\rho_S(0)] = \hat{\Lambda}_t^{Kraus}[\rho_S(0)] + \varpi(t), \quad (3.28)$$

where $\hat{\Lambda}_t^{Kraus}$ is a completely positive map given by equation (3.19), and the inhomogeneous term $\varpi(t)$ depends on the choice of a particular $\rho_T(0)$, see equation (3.25), and reads

$$\varpi(t) = \text{Tr}_E \left\{ U_t (\rho_T - \rho_S \otimes \rho_E) U_t^\dagger \right\}.$$

Notice that $\varpi(t)$ is Hermitian and traceless, i.e. $\text{Tr}_S \{\varpi(t)\} = 0$. We must also emphasize that the state $\rho_T(0)$ does not need to be such that $\text{Tr}_E \{\rho_T(0)\} = \rho_S(0)$ for every $\rho_S(0)$. Quite the contrary, what we want is just one particular choice of $\rho_T(0)$ and then generalize the resulting map to every state $\rho_S(0) \in S(\mathfrak{A})$.

Some quick comments about the map \hat{M} are in order. First, let us observe the trivial fact that there are no *a priori* restrictions on its domain of definition, that is $\text{dom} \{\hat{M}\} = \mathfrak{B}(\mathfrak{H})$. What is more, the affine map preserves the convex structure of $S(\mathfrak{A})$ in the sense that

$$\hat{M} \left[p\rho_S^{(1)} + (1-p)\rho_S^{(2)} \right] = p\hat{M} \left[\rho_S^{(1)} \right] + (1-p)\hat{M} \left[\rho_S^{(2)} \right], \quad \forall \rho_S^{(1)}, \rho_S^{(2)} \in S(\mathfrak{A}).$$

However, there is no reason why one should expect that the image of $S(\mathfrak{A})$ under the action of every \hat{M} of the form (3.28) should be contained in $S(\mathfrak{A})$ itself. To see this suppose that the map is defined such that there exists a pure state, Ψ_S , which is a fixed point of Λ_t^{Kraus} ; that is $\Lambda_t^{Kraus}\Psi_S = \Psi_S$ (an example of such a map is given in section 5.6). Thus, the map would yield $\hat{M}_t[\Psi_S] = \Psi_S + \varpi(t)$ which, in general, is not an element of $S(\mathfrak{A})$ (it is easy to convince oneself that the combination of a pure state and a non-zero traceless Hermitian operator will not be a density matrix in general, it would violate the positivity condition). But this is not surprising since the map \hat{M} is built out of the evolution of an initially correlated state of S and E , which is incompatible with $\rho_S(0)$ being a pure state. In fact if we took a pragmatic attitude and assumed that any physical realization of the map is of the form of a unitary evolution of $\rho_T(0)$, which has been our philosophy throughout the chapter, then it is irrelevant to study the action of anything but a completely positive map on a $\rho_S(0)$ which is pure (if anything, the study of the effect of a map of the form of \hat{M} on a pure state would only be a mathematical curiosity).

Therefore, using the notation of section 1.2, we have that $\text{range} \{\hat{M}|_{S(\mathfrak{A})}\} \subset \mathfrak{B}(\mathfrak{H})$, but, in the general case, $\text{range} \{\hat{M}|_{S(\mathfrak{A})}\} \not\subset S(\mathfrak{A})$. Nevertheless, notice that by definition there is at least one state ρ_S whose image under \hat{M} is another (physical) state, namely the one derived from the particular ρ_T used in the definition of $\varpi(t)$; hence $\text{range} \{\hat{M}|_{S(\mathfrak{A})}\} \cap S(\mathfrak{A}) \neq \emptyset$. What is more, it is reasonable to suppose that there exists a set $\tilde{A} \subset S(\mathfrak{A})$, that is not a singleton and that we will call the *positivity domain*, such that $\text{range} \{\hat{M}|_{\tilde{A}}\} \subset S(\mathfrak{A})$. Some of the elements belonging to \tilde{A} will be all the states ρ_S that are *compatible* with the values of $\gamma_{i\nu}$ used in the definition of $\varpi(t)$, that is, all the states $\rho_S = \text{Tr}_E \{\rho_T\}$ for whom their particular ρ_T results in a given $\gamma_{i\nu}$.

Recently, [Jordan *et al.* 2004] studied the structure of the positivity domain \tilde{A} (although they formulated their problem, and the map, somewhat differently), for the particular case where both S and E were each a qubit. For their example they calculated what were the possible states ρ_S compatible with a given $\gamma_{i\nu}$, however they also found that there are other states in \tilde{A} but that these depend on time. In other words, they found states that result from ρ_T 's that do not coincide with $\gamma_{i\nu}$, but are nevertheless transformed into proper states under the action of \hat{M}_t for particular values of t .

In section 5.7 we make a brief study of the positivity domain of a generalized depolarizing map. We have not tried to study the conditions for the elements of \tilde{A} for more general maps since the characterization of positive (but not completely positive) maps is quite difficult and remains an open problem [Zyczkowski & Bengtsson 2004]. For our purposes the only worthwhile result is that we know that a map, \hat{G} , that preserves Hermiticity for every state operator can

always be decomposed as

$$\hat{G}\rho = \sum_{i=1}^{m-1} C_i \rho C_i^\dagger - \sum_{j=m}^N B_j \rho B_j^\dagger.$$

This result has been rediscovered several times, but using very different techniques, by [Yu 2000], [Sudarshan & Shaji 2002], and [Royer 2005].

Thus, if a map is to preserve positivity for every state then it certainly needs to preserve Hermiticity. However, it is easy to convince oneself that, in general, $\hat{G}\rho \notin S(\mathfrak{A})$; even if the map is chosen so as to preserve the trace, i.e. $\sum_{i=1}^{m-1} C_i^\dagger C_i - \sum_{j=m}^N B_j^\dagger B_j = \mathbf{1}$. Hence, if \hat{G} is to map a density matrix to another density matrix this will only be achievable over a restricted set of $S(\mathfrak{A})$.

The previous paragraphs lead us to question the range of validity of applying a unique *linear* map (not to mention completely positive), $\hat{\Lambda}_t$, to every ρ in $S(\mathfrak{A})$. We saw that the existence of initial correlations between the system of interest and the environment can result in non-completely-positive transformations of the state of S , which if we try to extend to the whole of $S(\mathfrak{A})$ risks producing unphysical states. Furthermore, simply the idea that a dynamical map forms a semigroup seems to depend on the existence of an uncorrelated initial state [Royer 1996] [Burghardt 2001], which given our previous comments would appear to require a weak coupling with the environment. In fact, if there is a weak coupling one can show that the effect of the initial correlations will quickly die out and the inhomogeneous term in the Nakajima-Zwanzig equation will vanish [Facchi *et al.* 2005]. (This factorizing or weak-coupling condition is distinct from the conditions related to Markovian dynamics which are usually a property solely attributed to the environment. Yet, even for the Markovian assumptions, one has to take care about the possible influence the system of interest can have upon the environment [Presutti *et al.* 1972] [Fain 2000]).

These considerations leave us in a very uncomfortable position when trying to deal with open quantum systems if we do not have access to global observables allowing us to distinguish an initially uncorrelated state from a correlated one. Whether a preparation procedure breaks any initial correlations between S and E is debatable; it would seem that to do this would require an exquisite level of control on part of the experimentalist (which is not always the case). As well, we should expect that initial correlation effects should be relevant in non-Markovian systems, i.e. in situations where the system of interest and the environment evolve in similar time scales. This scenario is exemplified by solute-solvent dynamics as experimentally observed on the femtosecond time scale [Mukamel 1995] [Hamm *et al.* 1998]. However, as we saw, the existence of specific correlations between S and E in the initial state of the total system means accepting that in certain cases the reduced dynamics of the system of interest are only properly defined on a subset of possible states of S . Still, experimentalists should not be surprised by this, since in practice they usually only study a subset of states, namely those not too far out from equilibrium. In fact, theorists should also not be too surprised by a restriction to a certain region of state space since whenever they approximate the Hilbert space of the system to one of finite dimension they are usually limiting themselves to a given subset of states out of all the ones that can potentially exist. In sections 4.2 and 5.7 we will have to deal with situations where it will be inevitable to restrict ourselves to a subset of states to obtain physical results.

3.6 Stochastic differential equations and other methods

There are still a multitude of other methods for dealing with quantum systems that we have not mentioned (and that we will not use in this thesis). For example we have not written anything about the use of the machinery of path integrals. In this context the dynamical map $\hat{\Lambda}_t$ is called the influence functional and was first introduced by [Feynman & Vernon 1963]. However this method, as originally formulated, is only valid for factorized initial conditions [Hu *et al.* 1992].

As well, for a system of interest with continuous degrees of freedom, it is common practice to transform the density matrix into a Wigner function (see section 1.5.2) and then write out the master equation for this new quantity. The resulting equations of motion usually take the general form of the Fokker-Planck equation [Risken 1989] and are sometimes referred to as Weyl-Wigner-Moyal dynamics [Isar *et al.* 1994].

Also, several authors modify the equations of motion so as to obtain stochastic differential equations [Breuer & Petruccione 2002]. For example, in the Heisenberg picture one can add stochastic terms to the usual equation obtained for an observable from the von Neumann equation thus obtaining an effective Langevin equation [Haken 1970]. In the Schrödinger picture the technique usually involves supposing that the system described by ρ is formed by an ensemble of elementary systems each in a pure state that obeys a (typically non-linear) stochastic Schrödinger equation of the general form [Wiseman & Diósi 2001]:

$$|\dot{\psi}\rangle = -iH_\psi |\psi\rangle + \text{noise}_\psi,$$

where H_ψ is a non-Hermitian effective Hamiltonian which (like the noise) depends on ψ .

Using this stochastic differential equation one can perform so-called *unravellings* of the master equation; that is, the effective Hamiltonian and noise term are chosen such that the ensemble average coincides with the master equation describing the evolution of ρ . For example, for diffusive unravellings of an open system the equation is typically constructed such that its ensemble average coincides with the Lindblad equation, and it reads as [Breuer & Petruccione 2002]:

$$\begin{aligned} |d\psi\rangle = & -\frac{i}{\hbar}H|\psi\rangle dt + \sum_{\alpha} \left\{ 2\langle V_{\alpha}^{\dagger} \rangle_{\psi} V_{\alpha} - V_{\alpha}^{\dagger}V_{\alpha} - \langle V_{\alpha}^{\dagger} \rangle_{\psi} \langle V_{\alpha} \rangle_{\psi} \right\} |\psi\rangle dt \\ & + \sum_{\alpha} \left\{ V_{\alpha} - \langle V_{\alpha} \rangle_{\psi} \right\} |\psi\rangle d\xi_{\alpha} \end{aligned} \quad (3.29)$$

where the operators V_{α} are the same as those appearing in the Lindblad equation (3.23), and $\langle V_{\alpha} \rangle_{\psi} = \langle \psi | V_{\alpha} | \psi \rangle$. The $d\xi_{\alpha}$ are independent complex differential random variables representing a complex normalized Wiener process.

It is now important to mention that the stochastic Schrödinger equation (3.29) also appears in a somewhat different context from the one of open systems considered here. Namely, several authors have suggested the use of this type of equation as a stochastic model of the collapse of the wavefunction; see for example [GRW 1986], [Gisin & Percival 1992], and [Pearle 1993].

In the rest of this thesis, mainly due to practical reasons, we will not use any of the aforementioned methods, except for a brief mention of the stochastic Schrödinger equation (3.29) in section 6.4.3.

Chapter 4

Decoherence and the $Q \rightarrow C$ Transition

In this chapter we would like to cover the basics of decoherence theory as an explanation for the emergence of classical behaviour out of a quantum substrate. The first section is a short introduction, and critique, of the basics of decoherence. The second section provides an example of a simple model system capable of exhibiting ideal decoherence, but we will show how this can change if one considers initially correlated states (this will be the principal original contribution of the chapter).

4.1 The ideal decoherence programme

The decoherence programme is a very well established theory and it would be pretentious to try to make a new review when there already exist several good ones, some even by the original proponents of the theory [Zeh 2000] [Zurek 1991] [Zurek 2003]. However, although the original use of the term decoherence relates to attempts to understand the emergence of classical properties of quantum systems and to solve the quantum measurement problem through the dynamical interaction of the system of interest with an environment, the term nowadays has several different meanings depending on the context. For example, in the consistent histories and many-worlds interpretations of quantum mechanics it is also sometimes used for the apparent disappearance of coherent terms in coarse-grained descriptions of the state of the system without necessarily invoking an interaction with an environment [Gell-Mann & Hartle 1993] [Omnès 1994]. Therefore, since this thesis has a non-trivial intersection with decoherence theory, we would like to clarify what we will mean by this term.

The general idea behind decoherence is quite simple. It mainly consists in taking into account that the interaction of an open quantum system with its environment creates correlations between the two. After tracing over the environment's degrees of freedom, for particular types of interaction, a certain set of states of the open system will exhibit strong stability (the so-called einselection [Zurek 1998] and predictability sieve [Zurek 1993]) while the coherent superposition of these states is destroyed in the course of time.

In a variety of theoretical models it turns out that the environmental interaction leads to a decay of the coherence of such superpositions on extremely short time-scales, much shorter than the corresponding relaxation times of the open systems [Joos & Zeh 1985] [Zurek 1986] [Tegmark 1993] (For future reference it is important to point out that the models considered in all these articles assume initially uncorrelated states). Thus, the environment induces the

emergence of effective superselection sectors [Giulini *et al.* 1996]. The latter give rise to a decomposition of the reduced system's Hilbert space into coherent subspaces in such a way that coherent superpositions between different subspaces are no longer observable locally.

Several experiments have confirmed some of the basic tenets of decoherence in a number of physical systems. Some of the most notable examples are: [Brune *et al.* 1996] (microwave cavity), [Myatt *et al.* 2000] (trapped ions), [Hornberger *et al.* 2003] and [Hackermüller *et al.* 2004] (matter wave interferometry).

In its purest form, decoherence arises for certain types of $S - E$ interactions. These are (von Neumann) measurement-type interactions which are used to describe indirect measurements (see section 2.1) on the system of interest whereby the environment plays the rôle of the quantum probe.

The starting point of what we will call the *ideal* decoherence scheme is a Hamiltonian, for the total system, of the form

$$H_{S \cup E} = H_S + H_E + H_{SE}.$$

The key assumption behind ideal decoherence is that there exists a set of projectors $P_n^S = |n\rangle_S \langle n|$, forming a fine-grained partition of the Hilbert space of the system of interest S , that are conserved quantities; i.e:

$$[H_{S \cup E}, P_n^S \otimes \mathbf{1}_E] = 0. \quad (4.1)$$

Therefore, if this condition is satisfied, the complete set of orthonormal basis vectors $\{|n\rangle\}_n$ will be unaffected by the environment. The states $\{|n\rangle\}_n$ are usually called *pointer* states and their invariance is the main idea behind the concept of einselection and the predictability sieve.

The other main point about ideal decoherence is that the evolution of the total system is assumed to be of the general form:

$$U_t(|n\rangle_S \otimes |\phi\rangle_E) = |n\rangle_S \otimes (V_n(t) |\phi\rangle_E) = |n\rangle_S \otimes |\phi_n(t)\rangle_E \quad (4.2)$$

(see chapter 2 for examples of interactions resulting in this type of evolution). It is worth remembering that if there exists a global (additive) conserved quantity of the total system then the previous assumption will be restricted by the WAY theorem (see section 2.2).

Another common assumption in models of decoherence is that the initial state of the total system is uncorrelated and given by

$$\rho_T = |\psi(0)\rangle_S \langle \psi(0)| \otimes \rho_E(0),$$

with

$$|\psi(0)\rangle_S = \sum_n c_n |n\rangle_S. \quad (4.3)$$

Then, under the previous scenario of ideal decoherence, the reduced state of the system of interest will evolve into

$$\rho_S(t) = \sum_{nm} c_n \bar{c}_m |n\rangle_S \langle m| \text{Tr}_B \left\{ V_m^\dagger(t) V_n(t) \rho_E(0) \right\}.$$

Without any loss of generality let us define the decoherence function $\Gamma_{nm}(t)$ as

$$\Gamma_{nm}(t) = -\ln \left\{ \text{Tr}_B \left\{ V_m^\dagger(t) V_n(t) \rho_E(0) \right\} \right\}.$$

Obviously $\Gamma_{nm}(t) \geq 0$ for all times.

The time dependence of the decoherence function $\Gamma_{nm}(t)$ strongly depends, in general, on the properties of the underlying microscopic model ($H_{S \cup E}$) and on the choice of the initial state of the environment. Nevertheless, for many models it turns out that the off-diagonal components are severely damped (see [Breuer & Petruccione 2002] for a collection of the most typical examples). In fact, it is usually possible to define a characteristic decoherence time-scale, τ_{dec} , such that

$$e^{-\Gamma_{nm}(t)} \rightarrow \delta_{nm} \text{ for } t \gg \tau_{dec}.$$

Hence, if the microscopic Hamiltonian and the initial state of the environment do result in this behaviour, the resulting state of the system of interest will be

$$\rho_S(t) \rightarrow \sum_n P_n \rho_S(0) P_n = \sum_n |c_n|^2 P_n \text{ for } t \gg \tau_{dec}. \quad (4.4)$$

Thus, for times greater than the decoherence time-scale, the terms associated with the coherent superposition have disappeared. If we chose to define classicality with respect to the partition $\{P_n\}_n$ (see section 1.5.1) used above, we would have that

$$S(\mathfrak{A}) \rightarrow \tilde{C}_{\{P_n\}} \text{ for } t \gg \tau_{dec}.$$

In fact, this conclusion would also be valid if we changed our definition of classicality to the Abelian condition $[A, B] = 0$ for every $A, B \in \mathfrak{A}$. If we switched to the Heisenberg picture, the dynamical map associated with (4.4) would be

$$A(t) \rightarrow \sum_n P_n A(0) P_n \text{ for } t \gg \tau_{dec}.$$

And therefore we would have that, for times greater than the characteristic decoherence time-scale, the effective algebra of the system would be Abelian, viz. $[A(t), B(t)] = 0 \forall A, B$ for $t \gg \tau_{dec}$.

For the particular case of a fine-grained partition considered above, the state space of the system of interest is effectively split into one-dimensional superselection sectors (superpositions between these sectors are inhibited by the environment). However, the decoherence model also allows for higher-dimensional superselection sectors. For example suppose that the partition is coarse-grained (the associated observable is degenerate), and there exists a compatible observable whose eigenstates can be used to distinguish the degenerate states. In this case we could choose a coarse-grained partition of the form

$$P'_n = \sum_{j=1}^{d_n} |n, j\rangle_S \langle n, j|,$$

which, just as before, is assumed to be conserved, i.e. $[H_{S \cup E}, P'_n] = 0$.

For concreteness, let us choose an interaction term of the form $H_{SE} = \sum_n P'_n \otimes A_n^E$. Then an initially factorized state of the form

$$|\psi(0)\rangle_S \otimes |\phi\rangle_E = \sum_{n,j} c_{nj} |n, j\rangle_S \otimes |\phi\rangle_E,$$

would yield the reduced state of the system of interest

$$\rho_S(t) = \sum_{nm} \sum_{ij} c_{ni} \overline{c_{mj}} |n, i\rangle_S \langle m, j| \langle \phi_m(t) | \phi_n(t) \rangle.$$

In the limit of complete decoherence, $\langle \phi_m(t) | \phi_n(t) \rangle \rightarrow \delta_{nm}$, the state becomes

$$\rho_S(t) \rightarrow \sum_n \sum_{ij} c_{ni} \overline{c_{nj}} |n, i\rangle_S \langle n, j| \quad \text{for } t \gg \tau_{dec}.$$

Thus we see that in this case the superpositions between the state $|n, i\rangle_S$ for different i and a fixed n are still visible in the density matrix of the reduced system. This gives rise to an effective splitting of the Hilbert space of the system of interest, \mathfrak{H}_S , into superselection sectors such that

$$\mathfrak{H}_S = \bigoplus_n \{P'_n \mathfrak{H}_S\}.$$

It is perhaps important to mention here that this type of decomposition of the state space also occurs in settings different from the one of decoherence. For example [Wick et al. 1970] have postulated the existence of similar superselection sectors to explain the absence of superpositions of states with different charges. As well, superselection sectors arise naturally in many-body systems in the thermodynamic limit [Landsman 91] [Sewell 2002].

Although what we have defined as ideal decoherence is practically identical to an ideal von Neumann measurement, the philosophy and interpretation behind it is quite different. In particular, the arguments claiming that it helps to solve the quantum measurement problem involve assuming that the system of interest is composed of the system to be measured *and* the measuring apparatus [Zurek 1981]. Then, thanks to a tridecompositional theorem [Bub 1997], it is claimed that the einselection generated by the environment solves the problem of basis ambiguity in the quantum measurement problem. Nevertheless, to the best of our understanding, we do not see how decoherence could explain the appearance of a single outcome in each run of an experiment in a Copenhagen like interpretation. For other interpretations there is still a debate on whether decoherence solves the main issues. A detailed analysis of decoherence within the consistent histories interpretation has been given by [Kent & McElwaine 1997]. Discussions of the decoherence approach within the many-worlds interpretation can be found in [Bacciagaluppi 2001]. The most recent review of the application of decoherence theory to the quantum measurement problem, and of the main critiques, is [Schlosshauer 2004] (a shorter collection of arguments and references related to the shortcomings of decoherence for the measurement problem can be found in [Adler 2001]).

Regarding the adequacy of decoherence as an explication for the appearance of a classical world from a quantum substrate we believe the main critique involves the definition of classicality implied in decoherence theory (which coincides with our definition of classicality in section 1.5.1). In chapter 2 we have already presented various arguments against this definition. Even if we accepted this definition of classicality there are still several contentious assumptions in the decoherence programme, the most important of which we consider to be:

- How does one choose the system of interest in practice? This question also applies to the theory of open systems in general (even classical/Abelian ones). If the “system of interest”

is immersed in an environment with which it interacts it is not clear what is the correct definition of the variables that compose the system of interest (i.e. where does one separate the system of interest from the environment). This problem is even more pronounced in the case of many-body systems where, for example, it is common to work with quasi-particles [Bohm & Pines 1951], i.e. to dress the bare particles (the “original” system of interest) with what would otherwise normally be called the environment to obtain a redefined system of interest. This problem is not only relevant for macroscopic systems but also in the micro and mesoscopic regimes when some sort of organization emerges [Laughlin & Pines 2000] [Laughlin *et al.* 2000];

- Einselection. This is a “nice to have” property, both from the measurement and Q-C transition point of view, since it preserves the classical states (otherwise the bare unitary evolution would not preserve classicality). However, the assumption behind this is subject to several caveats. In the case of the existence of a globally conserved quantity einselection will be subject to the limitations imposed by the WAY theorem. Other aspects are studied in [Omnès 2002] where, in particular, he studies the consequences of relaxing the condition $[H_{S \cup E}, P_n] = 0$;
- The effectiveness of decoherence not only depends on the choice of the Hamiltonian (covered by the previous bullet) but also on the initial conditions. In particular, most models choose a factorized initial state of the total system, and even then they study very particular states of the environment (although, in general these are assumed to be states in thermal equilibrium which, if the factorized condition is valid, is not such an unreasonable assumption).

In the next section we will study a particular example of an ideal decoherence process and see how its properties are modified when one considers initially correlated states of the total system.

4.2 Decoherence and initial correlations

Suppose that the interaction with the environment is such that we have “ideal” decoherence in the case where the initial state of the total system is uncorrelated, i.e.

$$\begin{aligned} \rho(t) &= \text{Tr}_E \left\{ U_t (\rho(0) \otimes \rho_E(0)) U_t^\dagger \right\} \\ &= \hat{\Lambda}_t^{Zurek} [\rho(0)]. \end{aligned}$$

Then for times greater than the characteristic decoherence time-scale, $t \gg \tau_{dec}$, we should have (somewhat abusing the notation)

$$\lim_{t \gg \tau_{dec}} \rho(t) = \lim_{t \gg \tau_{dec}} \hat{\Lambda}_t^{Zurek} [\rho(0)] = \sum_n P_n \rho(0) P_n \quad \forall \rho(0) \in S(\mathfrak{A}).$$

In other words, it would seem that $\hat{\Lambda}_t^{Zurek}$, is such that $S(\mathfrak{A}) \rightarrow \tilde{C}_{\{P_n\}}$ as $t \gg \tau_{dec}$. However, as we saw in section 3.5, if $\rho_T(0) \neq \rho(0) \otimes \rho_E(0)$ (i.e. there exist initial correlations between the system of interest and the environment) then the evolution of the state of the system of interest looks like

$$\rho(t) = \hat{\Lambda}_t^{Zurek} [\rho(0)] + \varpi(t), \quad (4.5)$$

where $\varpi(t)$ is a traceless Hermitian operator. In the region of time where decoherence sets in we would have

$$\lim_{t \gg \tau_{dec}} \rho(t) = \sum_n P_n \rho(0) P_n + \lim_{t \gg \tau_{dec}} \varpi(t),$$

This expression can be suggestively recast into

$$\rho = \rho_C + \Pi_Q,$$

which would seem to imply that, if $\lim_{t \gg \tau_{dec}} \varpi(t) \neq 0$, the existence of initial correlations can spoil the main objective of decoherence, and, even more, produce a Q-state out of an original C-state! (See definitions of Q and C states in section 1.5.1) This is particularly worrying since the assumption in the whole decoherence programme is that the environment is unobservable which in turns means we could not distinguish, *a priori*, a correlated state from an uncorrelated one. However, the difference between these two initial conditions, correlated and uncorrelated, apparently has serious implications on the appearance of a classical world (or of a quantum world for that matter).

The question then would be if it is realistic to expect $\lim_{t \gg \tau_{dec}} \varpi(t) \neq 0$ whenever the interaction with the environment, and the reduced state of the environment, are such that they lead to decoherence in the case of a factorized initial state. In the tradition of Aristotelian logic, if we take into consideration that the origins of decoherence lie in the creation of correlations between S and E , we could be tempted to conclude that the existence of any correlations in the initial state could only lead to an enhancement of the decoherence effect. But this argument can be fallacious. Loosely, the claims that decoherence occurs on a timescale much shorter than thermal relaxation or dissipation [Joos & Zeh 1985] [Zurek 1986] [Tegmark 1993] are related to the constraints of relaxation times arising from completely-positive dynamics (which are the only type of dynamics for initially uncorrelated states of the total system, and are the only ones considered in the articles performing this sort of claim). For example, as we saw in section 3.5, for a two-level system, completely positive dynamics imposes constraints of the Bloch form $\tau_{\perp} \leq 2\tau_{\parallel}$ (where τ_{\perp} is the off-diagonal relaxation time, and τ_{\parallel} corresponds to the the diagonal -thermal- relaxation time), which is consistent with the claim that decoherence is faster than thermal relaxation. However, as mentioned previously, the Bloch relation can cease to be valid in the case of strongly interacting systems, which in turn excludes the possibility of an uncorrelated initial states. Thus, it would seem that there are enough precedents to suppose, contrary to our intuition, that initial correlations could actually counteract the decoherence effect we would otherwise obtain from an initially uncorrelated state.

In the next sections we will consider some examples that will show how, for certain conditions, the existence of initial correlations can actually reduce the “effectiveness” of decoherence, and in some extreme cases even result in the production of coherence.

4.2.1 Spin-boson model without initial correlations

To gain a better understanding of the effect that initial correlations can have on decoherence let us study the following instance of a simple spin-boson system which, for initially uncorrelated states, is one of the few analytically solvable models for decoherence. Before embarking on the correlated case we will review some of the known results of the uncorrelated case so as to have a point of comparison (this will also allow us to introduce some of the tools we will need).

Our model consists of a two-level system (the system of interest), and an environment consisting of a collection of non-interacting harmonic oscillators. The Hamiltonian of the total system is taken to be:

$$H_T = \underbrace{\frac{1}{2}\omega_0\sigma_z}_{H_S} + \underbrace{\sum_k \omega_k a_k^\dagger a_k}_{H_E} + \underbrace{\sum_k \sigma_z \left(g_k a_k^\dagger + \bar{g}_k a_k \right)}_{H_{SE}}, \quad (4.6)$$

where as usual σ_z is the Pauli matrix in the z-direction, ω_0 is the energy spacing between the two levels, and k labels the environment modes with frequencies ω_k and bosonic annihilation operators a_k satisfying

$$[a_k, a_{k'}^\dagger] = \delta_{kk'}.$$

Observe that the system dynamics are such that they preserve the diagonal components in the z-representation since

$$[|\pm\rangle\langle\pm| \otimes \mathbf{1}_E, H_T] = 0, \quad (4.7)$$

where $|\pm\rangle$ denote the eigenvectors of σ_z . Therefore the model conforms to the ideal decoherence model where the *pointer basis* is given by the eigenvectors of σ_z . The Hamiltonian (4.6) has been used extensively in models of decoherence for quantum computers [Unruh 1995]. However, also notice that the conservation law (4.7) implies that this model is limited in the sense that it does not capture thermalization effects (the bare energy eigenstates are stationary).

As mentioned previously, the model is exactly solvable, and without going into unnecessary details which can be found in [Palma *et al.* 1996] and [Breuer & Petruccione 2002], the interaction picture unitary propagator, apart from an overall time-dependent scalar phase factor, reads:

$$U_t^I = \exp \left\{ \frac{1}{2} \sigma_z \sum_k \left(\alpha_k(t) a_k^\dagger - \overline{\alpha_k(t)} a_k \right) \right\},$$

with the scalar amplitudes

$$\alpha_k(t) = 2g_k \frac{1 - e^{i\omega_k t}}{\omega_k}.$$

Thus, in the interaction picture, the time evolution for an arbitrary environment state $|\phi\rangle_E$ is given by

$$U_t^I (|\pm\rangle \otimes |\phi\rangle_E) = |\pm\rangle \prod_k D \left(\pm \frac{\alpha_k(t)}{2} \right) |\phi\rangle_E := |\pm\rangle \otimes |\phi_\pm(t)\rangle_E,$$

where we have introduced the displacement operator

$$D(\alpha_k(t)) = \exp \left\{ \alpha_k(t) a_k^\dagger - \overline{\alpha_k(t)} a_k \right\}. \quad (4.8)$$

Hence, the interaction of the system of interest with its environment leads to correlations between the pointer states $|\pm\rangle$ and certain environment states $|\phi_\pm\rangle$.

For means of future comparison, let us suppose (as is usually done) that the initial state of the total system is factorizable:

$$\rho_T^{fac}(0) = \rho(0) \otimes \rho_E(\beta). \quad (4.9)$$

Furthermore, let us suppose that the environment is in thermal equilibrium at the inverse temperature $\beta = 1/k_B T$, and therefore its state is described by

$$\rho_E(\beta) = \frac{e^{-\beta H_E}}{Z_E(\beta)}, \quad (4.10)$$

where $Z_E(\beta)$ is the partition function of the isolated environment ($Z_E(\beta) = \text{Tr} \{e^{-\beta H_E}\}$).

Obviously the populations (diagonal terms) of $\rho(t)$ in the z -representation remain constant in time, whereas the evolution of the off-diagonal terms in the Schrödinger picture is given by

$$\rho_{+-}(t) = \rho_{+-}(0) \exp \{i\omega_0 t - \Gamma(t)\}.$$

In this case where the environment is in thermal equilibrium the decoherence function $\Gamma(t)$ is found to be

$$\begin{aligned} \Gamma(t) &= -\ln \text{Tr}_E \left\{ \rho_E(\beta) \exp \left\{ \sum_k \left(\alpha_k(t) a_k^\dagger - \overline{\alpha_k(t)} a_k \right) \right\} \right\} \\ &= \sum_k \frac{4|g_k|^2}{\omega_k^2} (1 - \cos \omega_k t) \cosh \left\{ \frac{\beta \omega_k}{2} \right\}. \end{aligned}$$

A more detailed expression of the decoherence function depends on our choice of the physical properties of the environment. Let us make some preliminary comments before making a particular choice for the examples we will study. First notice that if the environment consists of a single mode then there will always be oscillatory behaviour, and thus no proper decoherence (there will be revivals of the off-diagonal component, or recoherence). If there are two modes, there is still the possibility of a complete revival of coherence if the frequencies are congruent in the sense that there exist two integer number $n_1, n_2 \in \mathbb{N}$ such that $\frac{\omega_1}{\omega_2} = \frac{n_1}{n_2}$. In general if the environment contains a discrete number of modes we should expect that there exists a recurrence time (Poincaré cycle); although this recurrence time can be extremely long [Fain 2000]. Hence, since we are interested in the case of irreversible behaviour where decoherence is “permanent”, we will suppose that the environment is composed of a macroscopic number of modes (for example in the case of a harmonic crystal composed of N atoms there would be $3N$ modes) which are spaced such that it is valid to take the continuum limit.

If we introduce the density $f(\omega)$ of modes at frequency ω and define the spectral density as

$$J(\omega) = 4f(\omega) |g(\omega)|^2,$$

we can write the decoherence function in the continuum limit as

$$\Gamma(t) = \int d\omega J(\omega) \frac{(1 - \cos \omega t)}{\omega^2} \cosh \left\{ \frac{\beta \omega}{2} \right\}. \quad (4.11)$$

Furthermore the quantity $J(\omega)$ is in general characterized by a cutoff frequency whose specific value depends on the physical realization considered. For example, if the environment corresponds to a phonon field, the natural cutoff can be identified with the Debye frequency (or equivalently with the separation between lattice sites), which is a parameter readily obtained from measurements of the heat capacity of the crystal [Ashcroft & Mermin 1976]. In the case

of a harmonic crystal the concept of a cutoff frequency is quite natural, it arises because there exists a minimum separation between particles (lattice sites) which in turns means that the approximation of a collective wave-like motion only makes sense up to a certain frequency.

In what follows we will confine ourselves to the often used case where the coupling is of the form $|g(\omega)| \sim g\sqrt{\omega}$ and the spectral density is given by

$$J_d(\omega) = b_d \omega^d e^{-\omega/\omega_c},$$

where ω_c is the cutoff frequency, d is the physical dimension of the environment, and b_d is a constant with units of $(\text{time})^{d-1}$.

In one dimension, $d = 1$, it is possible to obtain an analytic expression for the decoherence function, denoted by Γ^{1d} , if we assume that $\hbar\omega_c \gg 1/\beta$ [Breuer & Petruccione 2002]. If we define the thermal relaxation time as $\tau_\beta = \hbar\beta$ the expression is:

$$\Gamma^{1d}(t) = b_1 \left(\frac{1}{2} \ln \{1 + \omega_c^2 t^2\} + \ln \left\{ \frac{\sinh \{t/\pi\tau_\beta\}}{t/\pi\tau_\beta} \right\} \right). \quad (4.12)$$

The first term arises from the vacuum fluctuations, while the second one is due to thermal ones. There are three clear regimes for this one dimensional decoherence function, mainly ($b_1 = 1$):

1. The short-time regime $t \ll 1/\omega_c$: $\Gamma^{1d}(t) \approx \frac{1}{2}\omega_c^2 t^2$;
2. The vacuum regime $1/\omega_c \ll t \ll \tau_\beta$: $\Gamma^{1d}(t) \approx \ln \{\omega_c t\}$;
3. The thermal regime $\tau_\beta \ll t$: $\Gamma^{1d}(t) \approx t/\tau_\beta$.

It is clear that the decoherence function $\Gamma^{1d}(t)$ is a strictly increasing function of time, thus yielding, for $t \gg \tau_\beta$, an exponential decay of the off-diagonal components of the system of interest. In fact, numerical integrations show that this decay is also present even when the condition $\hbar\omega_c \gg 1/\beta$ is not satisfied [Palma *et al.* 1996].

It is perhaps more interesting to consider the three dimensional case, $d = 3$, where the integral (4.11) can be evaluated exactly without the previous restrictions to obtain the three dimensional decoherence function Γ^{3d} [Palma *et al.* 1996]:

$$\begin{aligned} \Gamma^{3d}(t) &= \frac{b_3}{\tau_\beta^2} \left(2\zeta \left(2, \frac{1}{\tau_\beta\omega_c} \right) - \zeta \left(2, \frac{1}{\tau_\beta\omega_c} (1 + i\omega_c t) \right) - \zeta \left(2, \frac{1}{\tau_\beta\omega_c} (1 - i\omega_c t) \right) \right) \\ &\quad + \frac{b_3\omega_c^2}{2} \left(\frac{1}{(1 + i\omega_c t)^2} + \frac{1}{(1 - i\omega_c t)^2} - 2 \right), \end{aligned} \quad (4.13)$$

where $\zeta(x, y)$ is the generalized Riemann zeta function. It is worthwhile cautioning the reader when he or she is dealing with the function $\zeta(2, y)$ in the vicinity of $y \sim 0$. Formally one has that $\zeta(2, 0) = \zeta(2) \simeq 1.64493$, however $\lim_{y \rightarrow 0^+} \zeta(2, y) = \infty$! If one takes care in performing the limit (or evaluates the integral directly, which is easier) the decoherence function when the environment is initially in its ground state, denoted by Γ_{gnd}^{3d} , is:

$$\Gamma_{gnd}^{3d}(t) = \int d\omega J_3(\omega) \frac{(1 - \cos \omega t)}{\omega^2} \left(= \lim_{\beta \rightarrow \infty} \Gamma^{3d}(t, \beta) \right) \quad (4.14)$$

$$= -\frac{b_3\omega_c^2}{2} \left(\frac{1}{(1 + i\omega_c t)^2} + \frac{1}{(1 - i\omega_c t)^2} - 2 \right). \quad (4.15)$$

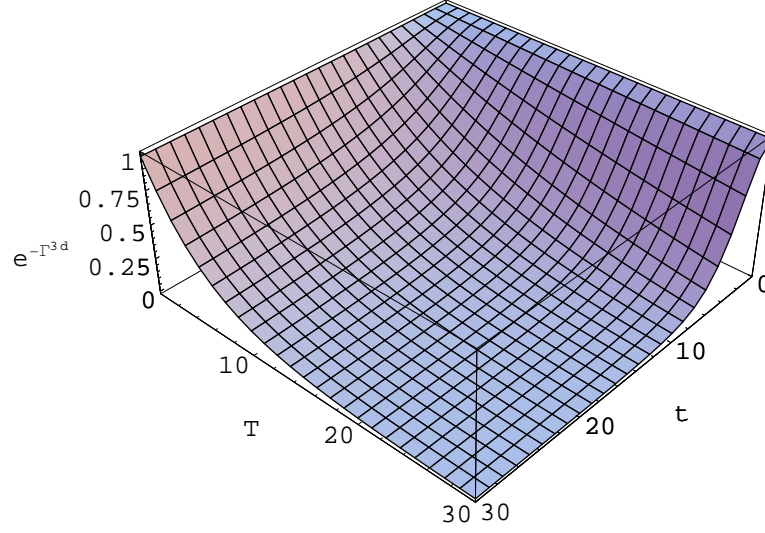


Figure 4.1: Plot of the decoherence factor $\exp\{-\Gamma^{3d}\}$ as a function of time and temperature for the cutoff frequency $\omega_c=0.1$ (temperature and frequency are in units such that $b_3 = 1$)

Notice the change in sign from what one would naively expect from simply setting $T = 0$ (i.e. $\tau_\beta \rightarrow \infty$) in (4.13).

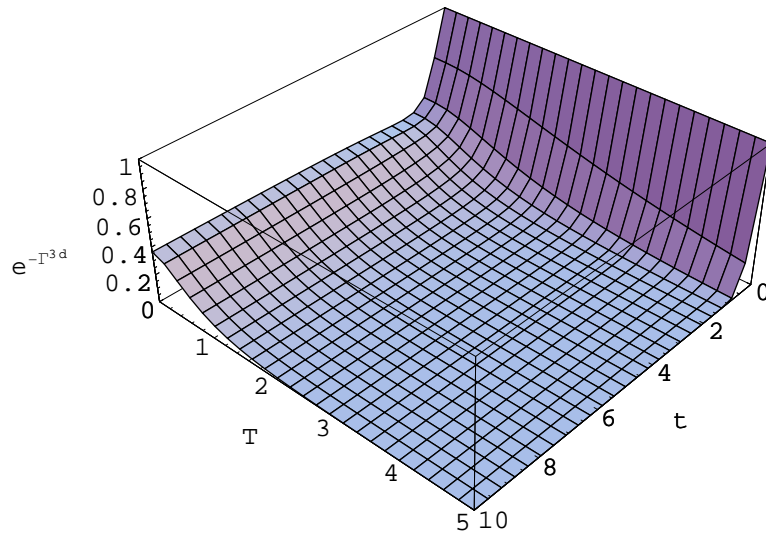
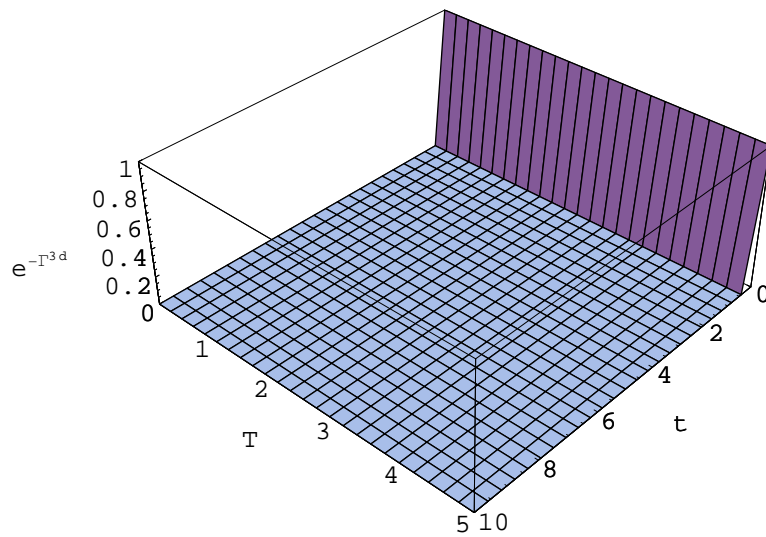
The three dimensional case definitely has a richer structure. Figures 4.1 to 4.3 show the behaviour of $\exp\{-\Gamma^{3d}(t)\}$ as a function of the temperature of the environment T ($= \hbar/k_B\tau_\beta$) and for various values of the cutoff frequency ω_c , both in units such that $b_3 = 1$. In particular, one can see that for certain values of T and ω_c the decoherence effect saturates. To see this let us take the limit of (4.13) when t is very large ($t \gg \tau_\beta$ and $t \gg 1/\omega_c$) to obtain:

$$\lim_{t \rightarrow \infty} \Gamma^{3d}(t) = b_3 \omega_c^2 \left(\frac{2}{\omega_c^2 \tau_\beta^2} \zeta \left(2, \frac{1}{\tau_\beta \omega_c} \right) - 1 \right). \quad (4.16)$$

Similarly the long time behaviour of the decoherence function when the environment is initially in the ground state is simply

$$\lim_{t \rightarrow \infty} \Gamma_{gnd}^{3d}(t) = b_3 \omega_c^2. \quad (4.17)$$

The point to consider is that in the three-dimensional case, for certain values of the temperature T and the cutoff frequency ω_c , the quantity $\lim_{t \rightarrow \infty} \Gamma^{3d}(t)$ can be sufficiently small so as to not result in complete decoherence (existence of residual coherence). This type of behaviour is reminiscent of the importance of dimensionality in phase transitions where, for short range interactions, the existence of long-range order is suppressed in one and two dimensional systems [Mermin & Wagner 1966] [Hohenberg 1967]. Figure 4.4 shows the behaviour of the quantity $c_q := \lim_{t \rightarrow \infty} \exp\{-\Gamma^{3d}(t)\}$ for $b_3 = 1$. The region where residual coherence is present is loosely characterized by $\hbar\omega_c \lesssim k_B T$. However, one needs to be careful since this regime will only be valid to a certain extent. For instance, if we return to the example of a harmonic crystal, it is possible to have $\hbar\omega_c \lesssim k_B T$, but at extremely high temperatures compared to ω_c the model will

Figure 4.2: Same as before, but for $\omega_c=1$.Figure 4.3: Same as above, but for $\omega_c=10$.

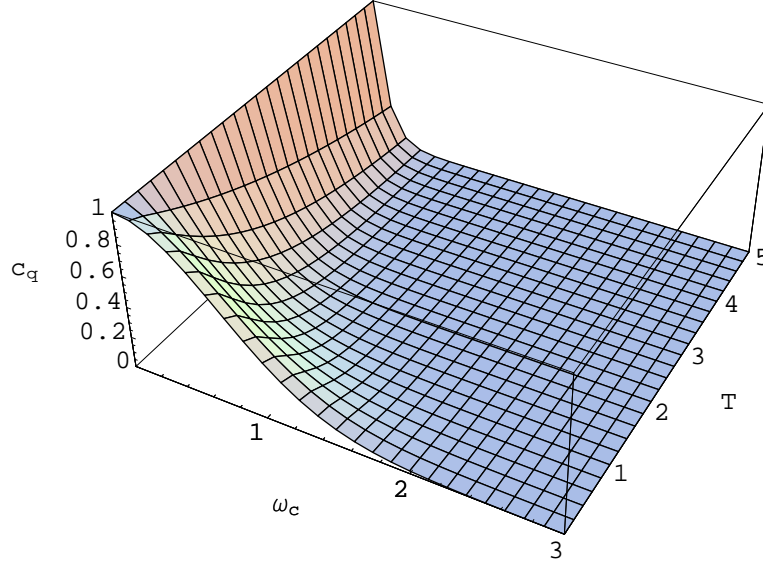


Figure 4.4: Plot of $c_q = \lim_{t \rightarrow \infty} \exp \{ -\Gamma^{3d}(t) \}$ as a function of the environment's temperature T and cutoff frequency ω_c .

break down (the crystal will melt) and it would make no sense to speak of a cutoff frequency, or at the very least its value will change. In the next sections the existence of these (decoherence) saturation regions will be shown to result in very interesting properties when we consider initially correlated states of the total system.

4.2.2 Initial correlations, decompositions, and positivity

The previous model, with a factorized initial condition, is well known in the literature. However, we have included it here because it can provide us with a tractable example to study the usually neglected consequences on decoherence due to the presence of initial correlations between S and E . To this end let us introduce some of the assumptions we will use to study the case where initial correlations are present.

First, let us suppose that the initial state of S is mixed (for there to be initial correlations the state of S must necessarily be so), and is given by:

$$\rho(0) = \text{Tr}_E \{ \rho_T(0) \} = \sum_{\mu=0}^M p_\mu \rho^{(\mu)}, \quad (4.18)$$

where $\sum_\mu p_\mu = 1$, and all the $\rho^{(\mu)}$ correspond to density matrices of the system of interest S .

Furthermore, let us consider the case when, at $t = 0$, S is classically correlated with E (this is the only case we will analyse), and therefore the density matrix of the total system can be written as:

$$\rho_T^{corr}(0) = \sum_{\mu=0}^M p_\mu \rho^{(\mu)} \otimes R_E^{(\mu)}, \quad (4.19)$$

with $R_E^{(\mu)}$ representing a valid state of the environment for every μ .

To make a sensible comparison with the initially factorized case (4.9) we will impose the restriction $\text{Tr}_S \{\rho_T(0)\} = \rho_E(\beta)$, where $\rho_E(\beta)$ coincides with the state of E given in (4.9), hence:

$$\sum_{\mu=0}^M p_\mu R_E^{(\mu)} = \rho_E(\beta). \quad (4.20)$$

Due to the properties of density matrices the state decompositions in (4.18), (4.19), and (4.20) can be highly degenerate [Hughston *et al.* 1993], therefore, to avoid complications that could cloud our objective, we will proceed as follows: We will suppose that we are given the explicit expressions for p_μ and $\rho^{(\mu)}$, such that they coincide with the state of the system of interest, $\rho(0)$, that is to be studied. As well, we will assume that the states $R_E^{(m)}$, with $m = 1, \dots, M$, are fixed and satisfy certain restrictions to be described in more detail below. Then, to satisfy the constraint (4.20) we will require that

$$R_E^{(0)} = \frac{1}{p_0} \left(\rho_E(\beta) - \sum_{m=1}^M p_m R_E^{(m)} \right). \quad (4.21)$$

These assumptions greatly simplify our problem since they assure us that the reduced states of our correlated state $\rho_T^{corr}(0)$ in (4.19) will coincide with the factors of $\rho_T^{fac}(0) = \rho(0) \otimes \rho_E(\beta)$, thus allowing us to make a proper comparison of the effects of initial correlations. Let us emphasize once more that if we only have access to local measurements on S and E independently then the states $\rho_T^{fac}(0)$ and $\rho_T^{corr}(0)$ are, *a priori*, experimentally indistinguishable. However, our simplification is not as trivial to execute as it may appear since we require $R_E^{(0)}$ to be a valid density matrix. From its definition in (4.21) it is obvious that $R_E^{(0)}$ is a Hermitian operator with $\text{Tr} \{R_E^{(0)}\} = 1$ (as long as every $R_E^{(m)}$ is a density matrix); but it is also clear that not every choice of $\{p_m R_E^{(m)}\}$ will result in a positive operator. This implies that the choice of the states $R_E^{(m)}$, and probabilities p_m , is not arbitrary. At the very least we should expect $\rho_E(\beta)$ to be more “mixed” than any of the constituents $R_E^{(m)}$ (this is easily inferred from the concave nature of the von Neumann entropy [Wehrl 1978]). Another basic requirement is that the density matrices $R_E^{(m)}$ need to satisfy:

$$\text{supp} \{R_E^{(m)}\} \subseteq \text{supp} \{\rho_E(\beta)\} \quad \forall m. \quad (4.22)$$

We will not try to establish a set of general criteria for the positivity of $R_E^{(0)}$, and for now we will accept that our choices of $\{p_m R_E^{(m)}\}$ give a positive $R_E^{(0)}$ (further on we will give some conditions for a particular example studied below).

One further assumption we will take for granted is that all the density matrices $\rho^{(m)}$ and $R_E^{(m)}$ in the decomposition of $\rho_T(0)$ are such that

$$\begin{aligned} \rho_{+-}^{(m)}(t) &: = \left\langle + \left| \text{Tr}_E \left\{ U_t \left(\rho^{(m)} \otimes R_E^{(m)} \right) U_t^\dagger \right\} \right| - \right\rangle \\ &= \rho_{+-}^{(m)} \exp \{ i\omega_0 t - \Gamma_m(t) \}, \end{aligned}$$

where, in the case of the spin-boson model under consideration, the decoherence term is given by

$$\Gamma_m(t) = -\ln \left\{ \text{Tr} \left\{ R_E^{(m)} \prod_k D(\alpha_k(t)) \right\} \right\}.$$

We will also accept that all the states $R_E^{(m)}$ satisfy $\Re \{\Gamma_m(t)\} \geq 0$ for all $t \geq 0$.

We will not be interested in the diagonal components since, from equation (4.7), it is trivial to see that no type of initial correlation will violate the conservation of these quantities.

With these assumptions we can get a glimpse of the effect of initial correlations. In the case where the initial state of the total system is factorized (equation 4.9), and the reduced state of the system of interest corresponds to the decomposition (4.18), the dynamics of the off-diagonal component will be given by:

$$\rho_{+-}^{fac}(t) = \left\langle + \left| \text{Tr}_E \left\{ U_t \rho_T^{fac} U_t^\dagger \right\} \right| - \right\rangle \quad (4.23)$$

$$= e^{i\omega_0 t - \Gamma(t)} \left(p_0 \rho_{+-}^{(0)} + \sum_{m=0}^M p_m \rho_{+-}^{(m)} \right), \quad (4.24)$$

with $\Gamma(t)$ given by equation (4.11).

However, if the initial state of the total system contains classical correlations between S and E of the type in (4.19), the dynamics of the off-diagonal component of the system of interest turn out to be

$$\begin{aligned} \rho_{+-}^{corr}(t) &= \left\langle + \left| \text{Tr}_E \left\{ U_t \rho_T^{corr} U_t^\dagger \right\} \right| - \right\rangle \\ &= e^{i\omega_0 t} \left(\rho_{+-}^{(0)} \left(e^{-\Gamma(t)} - \sum_{m=1}^M p_m e^{-\Gamma_m(t)} \right) + \sum_{m=1}^M p_m \rho_{+-}^{(m)} e^{-\Gamma_m(t)} \right). \end{aligned} \quad (4.25)$$

The difference between both situations, which are *a priori* indistinguishable if the observer only has access to local observables, is striking. The presence of initial correlations between the system of interest and the environment introduces a whole hierarchy of decoherence times. In the long run, the decay (if any!) of the “coherence” will be dominated by the environment component $R_E^{(m)}$ yielding the longest decoherence time. In fact, suppose that $\lim_{t \gg \tau_{dec}} e^{-\Gamma(t)} = 0$; if, as in the three-dimensional case, there exists a subset of environment states, denoted by the index $q \in \widetilde{ND}$, for which $\Gamma_q(t) \in \{\Gamma_m(t)\}_{m=1}^M$ satisfies $\exp\{-\Gamma_q(t)\} \sim c_q \neq 0$ for times t greater than some characteristic value $\tau_q \geq \tau_{dec}$ (and for which $\rho_{+-}^{(q)} \neq 0$), then the decoherence effect can, to some extent, be suppressed. In other words, if such states exist, and are present in the decomposition (4.20), we will have

$$\lim_{t \gg \tau_{no-dec}} \rho_{+-}^{corr}(t) = e^{i\omega_0 t} \left(\sum_{q \in \widetilde{ND}} p_q c_q \left(\rho_{+-}^{(q)} - \rho_{+-}^{(0)} \right) \right), \quad (4.26)$$

where we have defined $\tau_{no-dec} := \max_{q \in \widetilde{ND}} \{\tau_q\}$.

Since $\rho_{+-}^{(0)}$ and $\rho_{+-}^{(q)} \in [-1/2, 1/2]$, one can potentially have $(\rho_{+-}^{(q)} - \rho_{+-}^{(0)}) = \pm 1$ (this is supposing suitable values of the diagonal components of $\rho_{+-}^{(q)}$ and $\rho_{+-}^{(0)}$). Therefore, depending on the values of p_q and c_q (see equations 4.16 and 4.17), the long time value of $\rho_{+-}^{corr}(t)$ can be some non-negligible number. This implies that initial correlations can prevent the decoherence effect.

Nonetheless not everything is so nice and cosy. In the previous paragraph we have not dealt with any of the restrictions imposed by the requirement of a positive $R_E^{(0)}$ (which is something we require to be able to adhere to a statistical interpretation of the state). As we will see in the following example, the possible values of the probabilities p_m are strongly related to the decoherence functions $\Gamma_m(t)$, and to $\rho_E(\beta)$. This will show us that the residual coherence $\lim_{t \gg \tau_{no-dec}} \rho_{+-}^{corr}(t)$ will have an upper bound dependent on $\rho_E(\beta)$. Also, and perhaps more amazingly, is that equation (4.26) shows that our choice of the initial reduced state for S is not arbitrary, it depends on the properties of the environment (or the properties of the environment depend on the initial state of the system of interest). For the state of the system of interest to be positive we know that the off-diagonal components need to satisfy the bound:

$$|\rho_{+-}(t)| \leq \sqrt{\rho_{++}(1 - \rho_{++})} \quad \forall t,$$

which, if we consider the laxest scenario $|\rho_{+-}(t)| \leq 1/2$ for all t , would imply that

$$\sum_{q \in \widetilde{ND}} p_q c_q (\rho_{+-}^{(q)} - \rho_{+-}^{(0)}) \leq \frac{1}{2}.$$

This last relation shows that to ensure positivity of the state of S one needs either to impose a restriction on the possible (reduced) initial states of the system of interest S dependent on the environment parameters p_q and c_q , or alternatively, if one wants to allow any initial state of S then it is necessary to restrict the environment parameters p_q and c_q (i.e. the system of interest restricts the possible states of the environment). Nevertheless, this should not surprise us too much, there are other more general models of a two-level system interacting with a collection of bosons where the off-diagonal dynamics (tunneling rate) are related to the cut-off frequency of the boson system [Leggett *et al.* 1987, section III].

The previous analysis exemplifies the problem of studying initially correlated systems, and emphasizes the fact that, in addition to the initial state of the total system, one needs to consider the dynamics as well in the consideration of compatible initial states. What is more, it shows that for the system described by the Hamiltonian (4.6) in the continuum limit the quantity $\text{Tr}_E \left\{ U_t \rho_T U_t^\dagger \right\}$ does not always yield a positive matrix.

This last statement should surprise the reader. However, it seems that this is a pathology pervasive of infinite environments. There are several examples where, although the generator of the master equation (for an infinite environment) formally satisfies the trace preservation property, its solutions do not have a constant trace [Alicki 2002].

Before moving to the next section, and since we can no longer avoid talking about the conditions for the positivity of $R_E^{(0)}$, let us make some very specific assumptions about the type of correlations present in the initial state of the total system given in (4.19). In particular we

will suppose that the states $R_E^{(m)}$ (with $m \neq 0$) are pure, correspond to eigenvectors of $\rho_E(\beta)$ (or equivalently of H_E), and are distinct of each other; i.e. $R_E^{(m)} = |h_m\rangle\langle h_m|$ with

$$\rho_E(\beta) |h_m\rangle = h_m |h_m\rangle,$$

and

$$\langle h_m | h_{m'} \rangle = \delta_{mm'}.$$

In this particular case the conditions for the positivity of $R_E^{(0)}$ are especially simple. From the definition of $R_E^{(0)}$ in (4.21) it is easy to see that it will be positive if and only if the probabilities p_m satisfy the condition

$$p_m \leq \langle h_m | \rho_E(\beta) | h_m \rangle \quad \forall m.$$

Intuitively we would expect that if there are any states $|h_q\rangle$ such that $\lim_{t \rightarrow \infty} e^{-\Gamma_q(t)} \neq 0$, these would correspond to low energy eigenstates. This would seem to imply that, unless the environment is at a very low temperature, the probabilities p_q would be vanishingly small. However there are cases where this might not be so. For example, if the environment and its temperature are such that there is a Bose-Einstein condensate, the ground state will be macroscopically populated thus allowing for a non-negligible value of p_q . At any rate, we are still confronted with the fact that if $p_q \neq 0$ and $c_q \neq 0$ there is the potential for some residual coherence not present in the case where the initial state of the total system is factorizable. As mentioned before, this has non trivial implications on the positivity of the state of S .

4.2.3 Examples of decoherence damping and residual coherence

To make the previous points clearer let us consider a couple of examples. Given our previous comments, and since we are interested in providing examples that demonstrate how initial correlations can inhibit the decoherence phenomenon, and even result in some sort of residual coherence non-existent in the initially factorized case, let us limit our discussion to a qualitative description where the chosen time units are such that all constants (b_1 , b_3 , and g) are set to one and to the case where the initial state of the total system is given by

$$\rho_T^{corr}(0) = p\rho^0 \otimes R_E^{(0)} + (1-p)\rho^V \otimes |\Omega_E\rangle\langle\Omega_E|, \quad (4.27)$$

where $|\Omega_E\rangle$ is the ground state of the environment, and $R_E^{(0)}$ is set equal to

$$R_E^{(0)} = \frac{1}{p} (\rho_E(\beta) - (1-p) |\Omega_E\rangle\langle\Omega_E|).$$

To ensure the positivity of $R_E^{(0)}$ we require that

$$(1-p) \leq \langle \Omega_E | \rho_E(\beta) | \Omega_E \rangle := p_\Omega.$$

To be consistent with the expressions for the decoherence functions Γ in section 4.2.1, we will calculate the ground state population of the boson bath as

$$p_\Omega = \frac{1}{Z_E(\beta)} = \exp \left\{ \int d\omega \frac{b_d}{4g} \omega^{d-1} e^{-\omega/\omega_c} \log \left\{ 1 - e^{-\beta\hbar\omega} \right\} \right\}.$$

Then, in the case of initial correlations between S and E of the type in (4.27), we have that the off-diagonal component of the system of interest will behave as

$$\rho_{+-}^{corr}(t) = e^{i\omega_0 t} \left(\rho_{+-}^0 \left(e^{-\Gamma(t)} - (1-p) e^{-\Gamma_{gnd}(t)} \right) + (1-p) \rho_{+-}^V e^{-\Gamma_{gnd}(t)} \right), \quad (4.28)$$

where Γ is the decoherence function when the environment is in the thermal equilibrium state $\rho_E(\beta)$, and Γ_{gnd} is the decoherence function when the environment is in its ground state $|\Omega_E\rangle\langle\Omega_E|$.

This needs to be contrasted with what would be obtained in the case of an initially factorized state $\rho_T^{fac}(0) = \rho(0) \otimes \rho_E(\beta)$ (with $\rho(0) = \text{Tr}_E \{\rho_T^{corr}(0)\}$ and $\rho_E(\beta) = \text{Tr}_S \{\rho_T^{corr}(0)\}$), viz:

$$\rho_{+-}^{fac}(t) = e^{i\omega_0 t - \Gamma(t)} (\rho_{+-}^0 + (1-p) \rho_{+-}^V). \quad (4.29)$$

Because we will only be interested in illustrating some of the extreme consequences of initial correlations in what follows all our examples will suppose that $\rho_{++}^0 = 1/2$ ($\rho_{--}^0 = 1/2$) and $\rho_{++}^V = 1/2$ ($\rho_{--}^V = 1/2$). This will allow us to consider initial states with ρ_{+-}^0 and/or ρ_{+-}^V equal to $\pm 1/2$.

As can be inferred from section 4.2.1, the dynamics will depend on the dimensionality of the environment. Let us focus first on the one-dimensional case, and let us limit ourselves to the regime $\hbar\omega_c \gg 1/\beta$. Then, by substituting the analytic expression for the decoherence function, equation (4.12), into (4.28) we find that in the case of an initially correlated state the off-diagonal term behaves as (with $b_1 = 1$):

$$\rho_{+-}^{corr-1d}(t) = e^{i\omega_0 t} \left(\rho_{+-}^0 \left(e^{-\Gamma^{1d}(t)} - (1-p) \frac{1}{\sqrt{1 + \omega_c^2 t^2}} \right) + (1-p) \rho_{+-}^V \frac{1}{\sqrt{1 + \omega_c^2 t^2}} \right).$$

By performing the necessary expansions it is easy to see that in the short-time ($t \ll 1/\omega_c \ll \tau_\beta$) and vacuum regime ($1/\omega_c \ll t \ll \tau_\beta$) the correlated and uncorrelated initial states are practically indistinguishable. It is only in the thermal regime ($1/\omega_c \ll \tau_\beta \ll t$) that the existence of initial correlations makes itself evident. In this (thermal) regime the dynamics can be approximated as:

$$\rho_{+-}^{corr-1d}(t) = e^{i\omega_0 t} \left(\rho_{+-}^0 \left(e^{-t/\tau_\beta} - (1-p) \frac{1}{\omega_c t} \right) + (1-p) \rho_{+-}^V \frac{1}{\omega_c t} \right).$$

However, even in this case the difference between the initially correlated and uncorrelated cases will be minute since the above approximation assumes $1 \ll \omega_c t$. Also, for sufficiently long times both, the initially correlated and uncorrelated cases, will decay to zero. Figure 4.5 shows an example of the decay of $\rho_{+-}(t)$ for both the initially correlated and uncorrelated cases, each yielding the same reduced states for the system of interest and for the environment (for clarity we have neglected the oscillatory term $e^{i\omega_0 t}$). As expected, the only region where there is an observable difference is in the vicinity of $t \sim \tau_\beta$, and for times larger than τ_β both cases result in complete decoherence.

Now let us consider the three dimensional case. If we substitute the expressions for the three dimensional decoherence functions, equations (4.13) and (4.14), we obtain

$$\rho_{+-}^{corr-3d}(t) = e^{i\omega_0 t} \left(\rho_{+-}^0 \left(e^{-\Gamma^{3d}(t)} - (1-p) e^{-\Gamma_{gnd}^{3d}(t)} \right) + (1-p) \rho_{+-}^V e^{-\Gamma_{gnd}^{3d}(t)} \right).$$

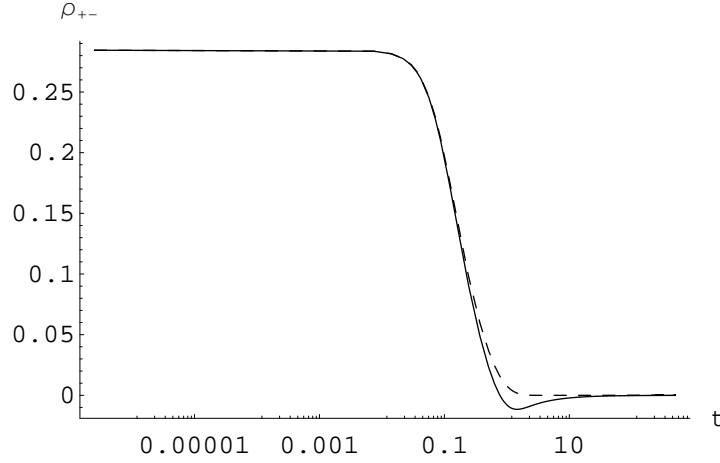


Figure 4.5: Semilogarithmic plot of $\rho_{+-}(t)$ in the one-dimensional case for both an initially correlated (solid line) and uncorrelated (dashed line) state of the total system yielding the same reduced states of S and E . The parameters used are $\tau_\beta = 1$, $\omega_c = 10$, $(1 - p) = p_\Omega = 0.21554$, $\rho_{+-}^0 = 0.5$, and $\rho_{+-}^V = -0.5$ (for clarity we have neglected the oscillatory term $e^{i\omega_0 t}$).

For most values of the temperature T and cutoff frequency ω_c there is no noticeable difference between the correlated and uncorrelated cases (this is because either the decoherence functions are very similar or the ground state probability p_Ω is too small for there to be any significant correlations in our model). However, as can be inferred from figure 4.4 at the end of section 4.2.1, there is a certain region of values where, in the long time regime, the thermal decoherence function, $\Gamma^{3d}(t)$, results in complete decoherence whilst the vacuum function $\Gamma_{gnd}^{3d}(t)$ saturates and results in a residual coherence. This will be the case we are interested in since this will correspond to the range of validity of (4.26).

Figure 4.6 shows a comparison of the decay of $\rho_{+-}(t)$ for correlated and uncorrelated initial states and for particular values of T and ω_c within the range of interest. Observe how, just as in the one-dimensional case, both initial conditions start to differ only in the vicinity of $t \gtrsim \tau_\beta$. However, in contrast to the one-dimensional case, here the saturation effect of the ground state plays a dominant rôle in the long time behaviour of the dynamics. The existence of initial correlations between the system of interest and the ground state result in the survival of a non-negligible amount of coherence (of the opposite sign to the original value) which is not present in the uncorrelated situation.

It is important to emphasize, as mentioned before, that one needs to take care in the selection of the initial correlated state for certain values of T and ω_c . As an example, figure 4.7 shows a particular choice of parameters and initial conditions that result in a non-positive state ($\rho_{+-}(t) \geq 1/2$). However, if we accept that for this type of environment parameters there still exist some valid initial reduced states of the system of interest (see discussion of limited domains in section 3.5), then this behaviour can result in exactly the opposite of decoherence. Figure 4.8 shows a particular choice of parameters where the initial reduced state has no coherence, $\rho_{+-}(0) = 0$, but the presence of initial correlations between the system of interest and the environment result in the production, and maintenance, of coherent behaviour (and a valid, positive, state).

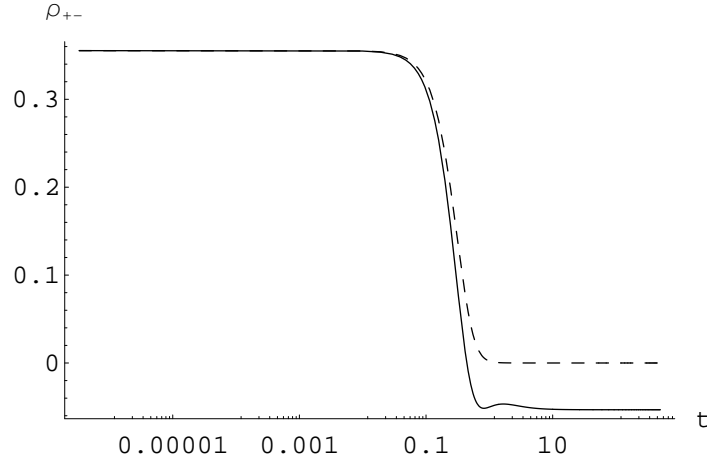


Figure 4.6: Semilogarithmic plot of $\rho_{+-}(t)$ in the three-dimensional case for both an initially correlated (solid line) and uncorrelated (dashed line) state of the total system yielding the same reduced states of S and E . The parameters used are $\tau_\beta = 0.2$, $\omega_c = 1$, $(1-p) = p_\Omega = 0.144613$, $\rho_{+-}^0 = 0.5$, and $\rho_{+-}^V = -0.5$ (for clarity we have neglected the oscillatory term $e^{i\omega_0 t}$).

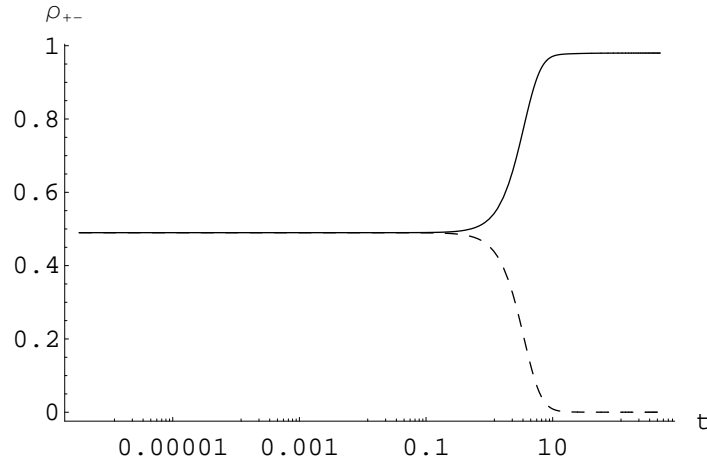


Figure 4.7: Example of a choice of an initially correlated state (solid line) resulting in a non-positive state for S . For comparison we have included the uncorrelated case (dashed line). The parameters used are $\tau_\beta = 0.025$, $\omega_c = 0.1$, $(1-p) = p_\Omega = 0.989906$, $\rho_{+-}^0 = -0.5$, and $\rho_{+-}^V = 0.5$ (for clarity we have neglected the oscillatory term $e^{i\omega_0 t}$).

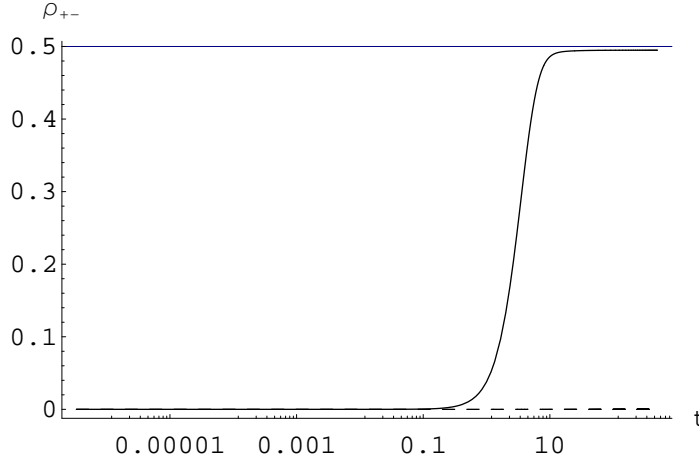


Figure 4.8: Example of how initial correlations between S and E can result in the creation of coherence instead of decoherence. The solid line corresponds to the initially correlated state, whereas the (constant) dashed line corresponds to the uncorrelated state. The parameters used are $\tau_\beta = 0.025$, $\omega_c = 0.1$, $(1 - p) = 0.5$ ($< p_\Omega = 0.989906$), $\rho_{+-}^0 = -0.5$, and $\rho_{+-}^V = 0.5$ (for clarity we have neglected the oscillatory term $e^{i\omega_0 t}$).

To summarize, we have shown that the existence of initial correlations can result in behaviour that is very different from that obtained by using an initially factorized state for the total system. In particular we have shown that, in the case of a three-dimensional environment, the presence of initial correlations can impair the decoherence effect even though both initial states (correlated and uncorrelated) are *a priori* indistinguishable if one only performs local measurements on S and E independently. Even more surprisingly we have seen that these initial correlations can even result in a net production of coherence. However, we must once again point out that for certain choices of the environment parameters not all initial states are valid, some will result in non-positive states. It is also important to note that all the examples in this section assumed units such that $b_d = 1$. Changing the value of this constant will affect the magnitude of the previous effects and/or shift the region of environment parameters where these “interesting” events take place, however the qualitative features will remain. It remains as future work to analyse a particular physical realization of the model used so as to fix the value of this constant and the other parameters.

Although the study of initial correlations has been severely neglected in the literature there are some previous results that seem to suggest that the effect of these initial conditions depends strongly on the given model. For example [Anglin *et al.* 1997] study the case of a Brownian oscillator (a harmonic oscillator coupled to an ohmic boson bath) and find that for the example they study, an initially entangled state, (in configuration space) the decoherence time can be much longer, but still always results in complete decoherence. This coincides with what is found in [Romero & Paz 1997] for the same model but for a class of more general initially correlated states. Similarly [Anastopoulos & Hu 2000], [Kofman 2001], and [Shresta *et al.* 2005] study a model of a two-level system coupled to a collection of bosons (however the interaction Hamiltonian they consider is different from ours) and find as well anomalously long decoherence times, but complete decoherence nonetheless. On the other hand [Bellomo *et al.* 2004] find that, for a free-particle

linearly coupled to a zero temperature bath of bosons, the decoherence in momentum space is complete and immediate in the case of initial correlations. This dependence of the effects of initial correlations on the particular model has been emphasized in the short-time regime by [Lutz 2003].

Nevertheless, we believe that our presentation here is the first report of an analysis of the effect of initial correlations, and a comparison of these to an “equivalent” factorized initial state (in the sense of having only access to local observables), for this particular model system which is often used for quantum computers. As well, none of the previous models has been shown to result in the curious residual coherence, coherence production, and restricted domain properties that appear in our model.

Chapter 5

Coherence Creating Processes

In this chapter we will study the often neglected case of how a system can perform a dynamical transition from classical to quantum behaviour, i.e. we will study the C→Q transition from a dynamical perspective.

In the previous chapter we already saw an example of how the interaction of the system of interest can, for a correlated initial condition, result in the production of a Q state. In this chapter, we would like to study under what conditions other types of transformations can result in the dynamical evolution from $\tilde{C}_{\{P_\mu\}}$ to $\tilde{Q}_{\{P_\mu\}}$. Along these lines we will pay special attention to the production of pure states from mixed ones.

5.1 Entropy considerations

In this (and the following) chapter we will be principally interested in processes that transform a mixed state into a pure one. In particular we will be interested in studying how can this be achieved by the interaction of a system with its environment. Before embarking on this study we would like to make some preliminary (and trivial) comments resulting from entropy considerations. Our main point will be that if the system of interest is to be purified it necessarily needs to dump its excess entropy into the environment (or somewhere else).

For our arguments we will use the von Neumann entropy defined to be [von Neumann 1932]:

$$S_{vN}[\rho] = -\text{Tr}\{\rho \ln \rho\}, \quad (5.1)$$

which is well known to be conserved under any unitary evolution, that is

$$S_{vN}[U\rho U^\dagger] = S_{vN}[\rho].$$

As mentioned at the beginning of chapter 3, the approach we will take when dealing with an open system is to suppose that the system of interest plus the environment obeys closed system dynamics, i.e. a unitary evolution. Therefore, if we suppose, without too much loss of generality (for the purposes of this chapter), that the initial state of the total universe (system of interest plus environment) is uncorrelated, i.e. $\rho_T(0) = \rho(0) \otimes \rho_E(0)$, then we would have that [Wehrl 1978]

$$S_{vN}[\rho(0)] + S_{vN}[\rho_E(0)] = S_{vN}[\rho_T(t)] \leq S_{vN}[\rho(t)] + S_{vN}[\rho_E(t)],$$

with the equality only occurring if $U_t \rho_T(0) U_t^\dagger = \rho(t) \otimes \rho_E(t)$ (as usual we have used the notation ρ_T , $\rho = \text{Tr}_E \{\rho_T\}$, and $\rho_E = \text{Tr}_S \{\rho_T\}$ to denote the state of the total system, the system of interest, and the environment respectively).

If the process results in a purification of the system of interest at time t , then the state of the composite system must be $\rho_T(t) = |\psi\rangle\langle\psi|(t) \otimes \rho_E(t)$. Since the entropy of a pure state is zero, we have that a purification process implies the relation

$$S_{vN}[\rho_E(t)] - S_{vN}[\rho_E(0)] = S_{vN}[\rho(0)]. \quad (5.2)$$

Thus, as expected, in a purification process the entropy of the environment increases by the quantity $S_{vN}[\rho(0)]$.

Now let us suppose that both the system of interest and the environment are of finite dimensions N_S and N_E respectively. It is easy to convince oneself that for an arbitrary system we always have

$$0 \leq S_{vN}[\rho_E(t)] \leq \ln N_E.$$

From the relation of entropy increase of the environment in the case of a purifying process, equation (5.2), we have that

$$0 \leq S_{vN}[\rho(0)] + S_{vN}[\rho_E(0)] \leq \ln N_E.$$

However, if we require our purification process to be also valid in the case that the initial state of the system of interest is the maximally mixed state $\rho(0) = \frac{1}{N_S}$, then

$$0 \leq S_{vN}[\rho_E(0)] \leq \ln \frac{N_E}{N_S};$$

which in turn implies

$$N_E \geq N_S.$$

To summarize, for a purification process to be realizable, the initial state of the environment needs to be such that it has enough capacity to absorb the excess entropy of the system of interest. Additionally, in the case of a finite dimensional universe, if the process is to be achievable for an arbitrary initial state of the system of interest then the dimension of the Hilbert space of the environment needs to be greater, or equal, than that of the system of interest.

5.2 Criteria for creating quantum coherence

Let us concentrate on the definition of classicality with respect to a given partition as introduced in section 1.5.1. The question we would like to address is: What are the properties a superoperator $\hat{\Lambda}_t$ should satisfy in order that it maps *any* classical state $\rho(0) \in \tilde{C}_{\{P_\mu\}}$ into a quantum state $\hat{\Lambda}_t \rho(0) \in \tilde{Q}_{\{P_\mu\}}$? We will call such a map a *coherence creating process* (CCP). Since we already have an example where a restricted map results in such a process (see section 4.2.3) we will be mainly interested in the case where the superoperator $\hat{\Lambda}$ maps every state into another state.

For simplicity we will only study the case where the system is of finite dimension N and the partition $\{P_\mu\}$ of the Hilbert space \mathfrak{H} is fine grained (i.e. the projectors of the partition are

one-dimensional). In this case, and for our purposes, it will be easier to express the operators belonging to $\mathfrak{B}(\mathfrak{H})$ using the canonical base $\{B_{\alpha=[ij]}\}_{\alpha=1}^{N^2} = \{|i\rangle\langle j|\}_{i,j=1}^N$ (see appendix A). Furthermore, the orthonormal basis $\{|i\rangle\}_{i=1}^N$ is chosen to coincide with the projectors with respect to which classicality is defined, i.e. $P_{\mu(=i)} = |i\rangle\langle i|$. Thus, using the usual notation $\rho_{ij} = \langle i|\rho|j\rangle$, any state $\rho \in S(\mathfrak{A})$ can be represented as

$$\rho \sim \vec{\rho} = \begin{pmatrix} \vec{c} \\ \vec{q} \end{pmatrix}, \quad (5.3)$$

where \vec{c} is a N -dimensional column vector composed of the diagonal elements of ρ , e.g.

$$\vec{c} = (\rho_{11}, \dots, \rho_{NN})^T, \quad (5.4)$$

and \vec{q} is a $(N^2 - N)$ -dimensional column vector composed of all the off-diagonal elements of ρ , e.g.

$$\vec{q} = (\rho_{12}, \rho_{21}, \dots, \rho_{N-1,N}, \rho_{N,N-1})^T. \quad (5.5)$$

In this representation the definition of the classical and quantum sets simplifies to

$$\tilde{C}_{\{P_\mu\}} = \{\rho | \rho \in S(\mathfrak{A}), \vec{q} = 0\},$$

and

$$\tilde{Q}_{\{P_\mu\}} = \{\rho | \rho \in S(\mathfrak{A}), \vec{q} \neq 0\}.$$

If we limit ourselves to the case where the actions of the maps are linear and defined over all $\mathfrak{B}(\mathfrak{H})$ (although, as we have seen in section 3.5, this is not the most general case), then they can also be conveniently decomposed in this representation as

$$\hat{\Lambda} \sim \begin{pmatrix} \Lambda_{CC} & \Lambda_{CQ} \\ \Lambda_{QC} & \Lambda_{QQ} \end{pmatrix}, \quad (5.6)$$

where Λ_{CC} , Λ_{CQ} , Λ_{QC} , and Λ_{QQ} are matrices of dimensions $N \times N$, $N \times (N^2 - N)$, $(N^2 - N) \times N$, and $(N^2 - N) \times (N^2 - N)$ respectively. For the choice of representation given in (5.4) and (5.5) the components are (with no summation over repeated indices):

$$\begin{aligned} (\Lambda_{CC})_{ii}^{mm} &= \text{Tr} \left\{ |i\rangle\langle i| \left(\hat{\Lambda} |m\rangle\langle m| \right) \right\}, \\ (\Lambda_{CQ})_{ii}^{mn} &= \text{Tr} \left\{ |i\rangle\langle i| \left(\hat{\Lambda} |m\rangle\langle n| \right) \right\}, \quad m \neq n, \\ (\Lambda_{QC})_{ij}^{mm} &= \text{Tr} \left\{ |j\rangle\langle i| \left(\hat{\Lambda} |m\rangle\langle m| \right) \right\}, \quad i \neq j, \\ (\Lambda_{QQ})_{ij}^{mn} &= \text{Tr} \left\{ |j\rangle\langle i| \left(\hat{\Lambda} |m\rangle\langle n| \right) \right\}, \quad i \neq j, m \neq n, \end{aligned}$$

all the indices i, j, m , and n run from 1 to N .

In this representation the question of the conditions for a CCP has a simple preliminary answer. Namely, the maps $\hat{\Lambda}$ taking any state $\rho(0) \in \tilde{C}_{\{P_\mu\}}$ (including the maximally mixed state $\rho = \frac{1}{N}$) to $\tilde{Q}_{\{P_\mu\}}$ are those for which $(\Lambda_{QC})_{ij}^{mm} \neq 0$ for every m . Conversely the condition to preserve classicality for all classical states is $\Lambda_{QC}(t) = 0$. (In fact, if we simply have that

$\Lambda_{QC}(t) \neq 0$, but not $(\Lambda_{QC})_{ij}^{mm} \neq 0$ for every m , then there will be some classical states that will remain classical while others will be transformed to Q-states).

Notice that Λ_{QC} is subject to a couple of restrictions inherited from $\hat{\Lambda}$, the most explicit of them is the one related to preserving Hermiticity, viz: $(\Lambda_{QC})_{ij}^{mm} = \overline{(\Lambda_{QC})_{ji}^{mm}}$. The trace preserving characteristics of $\hat{\Lambda}$ are solely encoded in Λ_{CC} and Λ_{CQ} , viz: $\sum_i (\Lambda_{CC})_{ii}^{mm} = 1$ and $\sum_i (\Lambda_{CQ})_{ii}^{mn} = 0$. The other restriction on Λ_{QC} , which we do not know how to write explicitly in the general case, arises from the conservation of the positive character of ρ (if we had an expression for this restriction, we would have a solution to the problem of characterizing positive, but not completely positive, maps; see discussion in section 3.5). Nevertheless, the positivity condition implies an interdependence between Λ_{QC} and the block matrices affecting the diagonal components, i.e. Λ_{CC} and Λ_{CQ} . The conditions related to positivity should be consistent with the “physical” restriction that $(\Lambda_{QC})_{ij}^{mm} = 0$ if $\rho_{ii}(t)$ or $\rho_{jj}(t) = 0$, i.e. we should not generate superpositions amongst non existent possibilities (see equation 1.14).

However $\Lambda_{QC}(t) \neq 0$ is not the end of the story of CCPs. First we have that the initial condition $\hat{\Lambda}(t=0) = \mathbf{1}$ implies that $\Lambda_{QC}(t=0) = 0$. Therefore, unless we are dealing with some sort of “violent” process (for example a collapse), we should only expect to obtain “measurable” coherences for times greater than some characteristic time scale, e.g. only for $t \geq \tau_{CCP} > 0$.

Also, notice that in general a unitary evolution for the system of interest will not in general preserve classicality (the only exception would be if the projectors in the partition $\{P_\mu\}$ are stationary, i.e. if they all commute with the effective Hamiltonian of the system of interest generating the unitary evolution). This would seem to make the question of finding CCPs rather trivial. However there are several comments to be made. First, it can be proven that, for a finite system, a unitary evolution will always be periodic [Scherer *et al.* 2004], therefore one should be more precise in defining the times or time interval for which the CCP should be present. Ideally we would like to find maps $\hat{\Lambda}$ that result in Q-states for intervals of time greater than the period of any associated unitary evolution. Secondly, a unitary evolution preserves the purity of the system, and given the discussion in section 2.6, and the fact that the most blatant Q-states are pure, what we would ideally like are maps that always yield pure states.

Therefore let us make a slight detour and focus on maps such that, for certain time intervals of interest, satisfy:

$$S(\mathfrak{A}) \xrightarrow{\hat{\Lambda}} \partial\tilde{Q}_{\{P_\mu\}}.$$

The effect of any map $\hat{\Lambda}_t$ (of the ones considered in this section) on $\rho(0) \in S(\mathfrak{A})$ can be written as

$$\rho_{ij}(t) = \sum_{m,n=1}^N (\Lambda_t)_{ij}^{mn} \rho_{mn}(0).$$

Our objective is to produce pure Q-states, this means that they should factorize as

$$\rho_{ij}(t) = \xi_i(t) \overline{\xi_j(t)}.$$

An ansatz for $\hat{\Lambda}$, denoted by $\hat{\Lambda}^{FixP}$, that would always yield this factorization is if its components also obeyed a factorization condition of the form:

$$\left(\hat{\Lambda}^{FixP}\right)_{ij}^{mn} = \alpha_i \overline{\alpha_j} \beta^{mn}. \quad (5.7)$$

From the conditions on page 34 for preserving Hermiticity and the trace, namely $\hat{\Lambda}_{nm,ij} = \overline{\hat{\Lambda}_{mn,ji}}$, and $\sum_n \hat{\Lambda}_{nn,qr} = \delta_{qr}$, we have that the β^{mn} term should be of the form:

$$\beta^{mn} = \frac{1}{\sum_{k=1}^N |\alpha_k|^2} \delta_{mn}.$$

Hence our ansatz becomes

$$\left(\hat{\Lambda}^{FixP}\right)_{ij}^{mn} = \frac{\alpha_i \bar{\alpha}_j}{\sum_{k=1}^N |\alpha_k|^2} \delta_{mn}. \quad (5.8)$$

It is easy to see that, since $\sum_m \rho_{mm} = 1$, this map will always result in a pure state, viz:

$$\forall \rho \in S(\mathfrak{A}), \quad \rho \xrightarrow{\Lambda^{FixP}} |\psi\rangle = \frac{1}{\sqrt{\sum_{k=1}^N |\alpha_k|^2}} \sum_{i=1}^N \alpha_i |i\rangle. \quad (5.9)$$

Moreover, as long as there are at least *two* distinct values of i and j such that $\alpha_i \neq 0$ and $\alpha_j \neq 0$, this pure state will belong to $\tilde{Q}_{\{P_\mu\}}$ (obviously if $\exists i \neq j$ such that α_i and $\alpha_j \neq 0$ then $\Lambda_{QC}^{FixP} \neq 0$). Also notice that the term δ_{mn} in (5.8) implies that the block matrices $\left(\hat{\Lambda}^{FixP}\right)_{CQ}$ and $\left(\hat{\Lambda}^{FixP}\right)_{QQ}$ only contain null components.

The drawback of $\hat{\Lambda}^{FixP}$ is that, although it can always produce a pure Q-state, this state is unique and independent of $\rho(0)$. (In the language of functional analysis $\hat{\Lambda}^{FixP}$ is a strict contraction over $S(\mathfrak{A})$ and therefore has a unique fixed point.) This means that the map is not compatible with Zurek's concept of a robust pointer basis which requires the existence of a set of extreme states that are unperturbed by the environment and that define the pointer basis [Zurek 1993].

In view of the previous let us consider the following scenario. Suppose we wanted to find a process that is the opposite of the ideal decoherence scheme (see section 4.1), i.e. a CCP $\hat{\Lambda}^Z$ that for every $\rho \in \tilde{C}_{\{P_\mu\}}$ generates off-diagonal elements but that preserves the diagonal elements (the vector \vec{c}). Such a process (for a typical norm of $\vec{\rho}$) would be a dilation of the vector $\vec{\rho}$. However, this gives us an insight into the difficulties of finding CCPs that yield pure states depending on the initial state. A system undergoing decoherence is going through a contraction of \vec{q} , this is naturally bounded by $\vec{q} = 0$ (however notice that there are an infinity of classical states ρ^C satisfying $\vec{q} = 0$). Thus, as long as one has a contraction one does not need to be too careful. Yet, a dilation process needs some special properties to ensure that \vec{q} does not “blow-up” since the conditions on ρ being a state imply that $\vec{q} \cdot \vec{q}^* \leq f(\vec{c})$, which in this example (of the exact opposite of ideal decoherence) is a constant upper bound.

Let us analyse this by pointing out that if there exists a map yielding a pure state whilst preserving the diagonal components of all C-states then the resulting state, ρ_{CCP} , of such a transformation can always be written as¹:

$$\rho_{\tilde{C}} = \sum_i p_i |i\rangle\langle i| \xrightarrow{\Lambda^Z} \rho_{CCP} = |\psi\rangle\langle\psi| = \sum_{ij} \frac{\sqrt{p_i p_j}}{\sqrt{\text{Tr}\{ |i\rangle\langle i| \Pi |j\rangle\langle j| \Pi \}}} |i\rangle\langle i| \Pi |j\rangle\langle j| \quad (5.10)$$

¹The expression for the pure state ρ_{CCP} given in equation (5.10) is based on the work in [Man'ko *et al.* 2002] where a similar construction was used to describe the coherent addition of pure states.

with $\Pi = |\varphi\rangle\langle\varphi|$. The amplitudes in the decomposition of $|\varphi\rangle$ are arbitrary but the phase relationships need to be the ones desired for ρ_{CCP} since

$$|\psi\rangle = \sum_i \sqrt{p_i} \frac{\langle i|\varphi\rangle}{|\langle i|\varphi\rangle|} |i\rangle. \quad (5.11)$$

The presence of the $\sqrt{p_i}$ terms on the rhs of (5.10) imply, in the general case, that if such a map were to exist then it necessarily would be *non-linear*. This is consistent with our previous comments about the special properties of the map so as to avoid a blow-up.

To better understand this let us concentrate on the case where $\vec{\rho}_Z(0) = (\vec{c}_Z, 0)^T$ with just two non-zero probabilities, e.g. $\vec{c}_Z = (\rho_{11}, \rho_{22}, 0, \dots, 0)^T$. In this case, if we want a CCP yielding a pure state with the same classical probabilities, we need a map with components such that its action on any $\rho(0) \in \tilde{C}_{\{P_\mu\}}$ (or at least for those of the form of \vec{c}_Z) gives

$$\rho_{12} = \sqrt{\rho_{11}\rho_{22}}e^{i\theta_{12}} = (\Lambda^Z)_{12}^{11}\rho_{11} + (\Lambda^Z)_{12}^{22}\rho_{22}$$

To achieve this the components of the map $\hat{\Lambda}^Z$ must obey the relationship

$$(\Lambda^Z)_{12}^{11} = \sqrt{\frac{\rho_{22}}{\rho_{11}}} \left(e^{i\theta_{12}} - (\Lambda^Z)_{12}^{22} \sqrt{\frac{\rho_{22}}{\rho_{11}}} \right). \quad (5.12)$$

This obviously would imply that $\hat{\Lambda}^Z$ is a *non-linear* map. What is more, this non-linearity is not only a peculiarity arising from trying to obtain pure states. Any map that takes an *arbitrary* classical state to a state in $\tilde{Q}_{\{P_\mu\}}$ while *preserving* the classical probabilities, i.e. a map generating off-diagonal terms but that preserves the diagonal ones, will necessarily be non-linear if it is to generate off-diagonal terms only when the associated diagonal elements are non-zero. (For the resulting state $\rho(t) = \Lambda_t \rho(0)$ to be physical we require that $\rho_{ij} = 0$ whenever $\rho_{ii} = 0$ or $\rho_{jj} = 0$).

Nonetheless the previous does not mean that for a given $\hat{\Lambda}$ there do not exist classical states that could be taken to pure Q-states whilst preserving its classical probabilities. For example in the case of the ansatz map $\hat{\Lambda}^{FixP}$ in (5.8), there exists a unique classical state, namely the one with components $\rho_{ii} = |\alpha_i|^2 / \sum_{k=1}^N |\alpha_k|^2$, that will be mapped to a pure state with conserved classical components.

The previous leads us to postulate that, in general, for a linear map $\hat{\Lambda}^{CCP}$ purification (for a large enough number of initial states) is only achievable via a fixed point evolution. An argument justifying this conjecture would run as follows:

Suppose that $\hat{\Lambda}^{CCP}$ actually purifies a particular mixed state ρ , i.e.

$$\hat{\Lambda}^{CCP} \rho = \Psi. \quad (5.13)$$

However, a mixed state can always be decomposed as

$$\rho = \sum_i p_i \Psi_i, \quad (5.14)$$

which coupled to the linearity assumption of $\hat{\Lambda}^{CCP}$ would imply that

$$\Psi = \sum_i p_i \hat{\Lambda}^{CCP} \Psi_i.$$

But by assumption Ψ is a pure state and therefore is an extreme point that cannot be decomposed in terms of other pure states (see section 1.4). Thus, the only way of satisfying (5.13) is if all the extreme states Ψ_i in (5.14) are mapped to the same state, viz:

$$\hat{\Lambda}^{CCP} \Psi_i = \Psi.$$

However we know that the decomposition in (5.14) is not unique [Hughston *et al.* 1993]. Thus, we have that there are several pure states that need to be mapped to a unique point Ψ . All the mixed states that can be decomposed in terms of all the possible pure states in the ensemble decomposition of ρ will also be transformed into Ψ . Therefore, if we were to require the purification of enough mixed states, whose ensemble decomposition have at least one pure state in common, then they would all need to be mapped to the fixed point Ψ . (By “enough” we should understand that the union of the supports of all these density matrices coincides with the entire Hilbert space, and that the set of these operators is such that one can always find another operator, in the set, such that the intersection of their supports is not empty).

To summarize, we have introduced a criterion for a linear map $\hat{\Lambda}$ to take C states into Q states. As well, we have introduced an ansatz for the general form of a map taking every mixed state to a pure state. However, we have also introduced a conjecture that if a linear map is to purify mixed states then this will only be achieved by taking all of the states to a unique extremal fixed point. Several of the ideas in this section will be studied further in the rest of the chapter.

5.3 Integro-differential equation for determining Q behaviour

Before continuing to a more concrete discussion of the C→Q transition we would like to quickly point out that if we are dealing with an open system obeying Markovian (semigroup) dynamics, and we know the structure of the master equation, then, at least in principle, we can determine if $\hat{\Lambda}(t)$ is a CCP, in the sense that $\Lambda_{QC} \neq 0$, without having to solve for all the components of $\hat{\Lambda}(t)$. To see this, notice that the assumption of semigroup dynamics means that $\hat{\Lambda}(t)$ obeys an equation of the form (see equation 3.23):

$$\frac{d}{dt} \hat{\Lambda}(t) = \hat{D} \hat{\Lambda}(t). \quad (5.15)$$

Using the representation (5.6) for the superoperator \hat{D} we can see that Λ_{QC} is only coupled to Λ_{CC} . The system of differential equations is

$$\frac{d}{dt} \Lambda_{CC} = D_{CC} \Lambda_{CC} + D_{CQ} \Lambda_{QC} \quad (5.16a)$$

$$\frac{d}{dt} \Lambda_{QC} = D_{QC} \Lambda_{CC} + D_{QQ} \Lambda_{QC} \quad (5.16b)$$

Taking advantage that D_{CC} and Λ_{CC} are square matrices we can formally integrate (5.16a) to obtain a closed equation for Λ_{QC} , viz:

$$\frac{d}{dt} \Lambda_{QC} = D_{QQ} \Lambda_{QC} + D_{QC} e^{tD_{CC}} + \int_0^t d\tau D_{QC} e^{(t-\tau)D_{CC}} D_{CQ} \Lambda_{QC}(\tau), \quad (5.17)$$

where we have used the boundary condition $\Lambda_{CC}(t=0) = 1_{N \times N}$. The initial condition for Λ_{QC} is $\Lambda_{QC}(t=0) = 0$.

This proves our point but it also shows part of the complication in trying to find a physical process (a master equation) leading to a CCP. Also, although we have obtained a closed equation for Λ_{QC} , it remains questionable whether this is the most productive way of analyzing the problem. In fact, one could argue that it is easier to solve the master equation for ρ (N^2 coupled differential equations) and vary the initial conditions, or even solve for the whole of $\hat{\Lambda}$ (N^4 coupled differential equations), instead of solving solely for Λ_{QC} ($N^3 - N^2$ coupled integro-differential equations). Because of this we will not use this equation in this thesis.

Also note that the similarity between our integro-differential equation (5.17) and the Nakajima-Zwanzig master equation in (3.2) is not gratuitous. The fact is that when performing the decomposition (5.6) of $\hat{\Lambda}$ into block matrices we have implicitly used (super-)projectors in much the same fashion as is done in the derivation of the Nakajima-Zwanzig master equation.

5.4 Universal non-Markovian CCP

Let us revisit the ansatz (5.8), viz:

$$\left(\hat{\Lambda}_t^{FixP}\right)_{ij}^{mn} = \alpha_i(t) \overline{\alpha_j(t)} \delta_{mn}, \quad (5.18)$$

(to ease the notation we have supposed that the coefficients $\alpha_i(t)$ are already normalized such that $\sum_{k=1}^N |\alpha_k|^2 = 1$). Our objective in this section is to construct a *non-Markovian completely positive map* with such properties and, if possible, to find a physical mechanism to produce it. (By non-Markovian we mean that we do not demand that the map satisfies the semigroup time composition property). Also let us note that in this section we will slightly change notation and denote the reduced state of the environment by σ_E instead of ρ_E .

As introduced in section 3.3, a completely positive map can always be decomposed as:

$$\hat{\Lambda}^{Kraus} = \sum_{\eta} \hat{L}_{W_{\eta}} \hat{R}_{W_{\eta}^{\dagger}}.$$

Which implies that its components are

$$\left(\hat{\Lambda}^{Kraus}\right)_{ij}^{mn} = \sum_{\eta} W_{im}^{\eta} \overline{W_{jn}^{\eta}},$$

with $W_{im}^{\eta} = \langle i | W_{\eta} | m \rangle$.

A possible choice for the generators W_{η} consistent with our ansatz (5.18) could be

$$W_{im}^{\eta} = \alpha_i \gamma_m^{\eta}, \quad (5.19)$$

subject to the (trace-preserving) condition

$$\sum_{\eta} \gamma_m^{\eta} \overline{\gamma_n^{\eta}} = \delta_{mn}. \quad (5.20)$$

So far we have not specified the range of the η index because we have some freedom in choosing it (in practice it is determined by the choice of the environment and its coupling with

the system of interest -although it can always be modelled/reduced to a representation with $\max\{\eta\} = N^2$). However let us now fix it such that its range coincides with the latin indices of the orthonormal basis $\{|i\rangle\}_{i=1}^N$ over the Hilbert space \mathfrak{H} of the system of interest (with respect to which we have defined classicality). Thus, a sensible choice for the Kraus operators consistent with (5.19) and (5.20) could be $\gamma_m^k = \langle k|V^\dagger|m\rangle$ leading us to:

$$W_k(t) = |\psi(t)\rangle\langle k|V^\dagger, \quad (5.21)$$

with $\{|k\rangle\}_{k=1}^N$ a complete orthonormal set over \mathfrak{H} , and V an arbitrary unitary operator. It is easy to see that this will achieve our objective, the generators $W_k(t)$ will transform any initial state $\rho(0)$ into a pure state $|\psi(t)\rangle$, viz:

$$\begin{aligned} \rho(t) &= \sum_{k=1}^N |\psi(t)\rangle\langle k|V^\dagger\rho(0)V|k\rangle\langle\psi(t)| \\ &= |\psi(t)\rangle\langle\psi(t)|\text{Tr}\{V^\dagger\rho(0)V\} \\ &= |\psi(t)\rangle\langle\psi(t)|. \end{aligned}$$

This extreme contraction of the whole state space to a single point obviously has strong implications for the evolution of observables in the Heisenberg picture. From the definition of the dual map for a completely positive map in (3.14) we have that for every $A \in \mathfrak{B}(\mathfrak{H})$ its time evolution is given by

$$\begin{aligned} A(t) &= \sum_{k=1}^N V|k\rangle\langle\psi(t)|A|\psi(t)\rangle\langle k|V^\dagger \\ &= \mathbf{1}\langle\psi(t)|A|\psi(t)\rangle. \end{aligned}$$

In other words the map resulting from our ansatz maps all the observables (in fact, all of the operators of the algebra) to the identity operator. Thus, our so-called CCP map results in an effective Abelian algebra which is quite the opposite of what we would expect from a map that in theory creates quantum coherence.

Now let us forget for a moment about our ansatz and suppose we did not know about the existence of Kraus generators such as the ones in (5.21). We want to study what are the consequences of requiring the factorization condition $\rho_{ij}(t) = \xi_i(t)\bar{\xi}_j(t)$ for *any* initial $\rho(0)$ when we consider the typical scenario where

$$\rho(t) = \text{Tr}_E \left\{ U_t(\rho(0) \otimes \sigma_E(0)) U_t^\dagger \right\} \quad (5.22)$$

As we saw in section 3.3 this assumption of an uncorrelated initial condition leads to the Kraus operators

$$W^{\alpha\beta}(t) = \sqrt{\lambda_\beta} \langle \varphi_\alpha | U_t | \varphi_\beta \rangle,$$

where $\{|\varphi_\beta\rangle\}_{\beta=1}^{N_E}$ is the orthonormal basis of \mathfrak{H}_E that diagonalizes the environment state $\sigma_E(0)$, namely $\sigma_E(0) = \sum_{\beta=1}^{N_E} \lambda_\beta |\varphi_\beta\rangle\langle\varphi_\beta|$. (Notice that we have changed notation and we have “split” the index η into $\alpha\beta$).

Thus, we are interested in determining the properties that the components

$$u_{im}^{\alpha\beta} = \langle i, \varphi_\alpha | U_t | m, \varphi_\beta \rangle$$

of the unitary evolution U_t need to obey in order for $\rho(t)$ to be a pure state.

A first guess could be that the components obey a relation of the form $u_{im}^{\alpha\beta} = f_i g_m^{\alpha\beta}$. However this is easily seen to be incompatible with the properties of U_t , since the unitarity condition would lead to the restriction $f_i \overline{f_j} \propto \delta_{ij}$ which is obviously unachievable. Other options, possibly consistent with the unitarity of U_t , could be $u_{im}^{\alpha\beta} = f_i^\alpha g_m^\beta$ or $u_{im}^{\alpha\beta} = f_{im}^\alpha g^\beta$, but these are incompatible with our objective of producing a pure $\rho(t)$. This stems from the fact that in the determination of $\rho(t)$ in the former case we are forced to sum over all α yielding terms like $\sum_{\alpha=1}^{N_E} f_i^\alpha \overline{f_j^\alpha}$ whilst in the latter we obtain terms of the form $\sum_{m,n=1}^{N_S} f_{im}^\alpha \overline{f_{jn}^\alpha} \rho_{mn}(0)$. Both cases are incompatible with the factorization of the components of a pure $\rho(t)$. Therefore, it seems that the only option yielding a pure state for an arbitrary initial $\rho(0)$ is if the unitary operator U_t has components obeying

$$u_{im}^{\alpha\beta} = f_i^\beta g_m^\alpha. \quad (5.23)$$

Nonetheless, if we are to attain our objective this assumption has to be coupled to an initial state of the environment that is pure!

Let us study further the case where U_t obeys (5.23), i.e.

$$U_t = \sum_{i,m=1}^{N_S} \sum_{\alpha,\beta=1}^{N_E} f_i^\beta g_m^\alpha |i, \varphi_\alpha\rangle \langle m, \varphi_\beta|. \quad (5.24)$$

(In what follows we can take $\{|i\rangle\}_{i=1}^{N_S}$ and $\{|\varphi_\alpha\rangle\}_{\alpha=1}^{N_E}$ to be arbitrary orthonormal basis, for \mathfrak{H}_S and \mathfrak{H}_E respectively, consistent with 5.23). The unitarity condition $U_t^\dagger U_t = \mathbf{1}_S \otimes \mathbf{1}_E$ implies the restrictions

$$\begin{aligned} \sum_{\alpha=1}^{N_E} g_m^\alpha \overline{g_n^\alpha} &= \delta_{mn}, \\ \sum_{\iota=1}^{N_S} f_i^\alpha \overline{f_\iota^\alpha} &= \delta_{\alpha\beta}; \end{aligned} \quad (5.25)$$

while $U_t U_t^\dagger = \mathbf{1}_S \otimes \mathbf{1}_E$ leads us to

$$\begin{aligned} \sum_{m=1}^{N_S} g_m^\alpha \overline{g_m^\beta} &= \delta_{\alpha\beta}, \\ \sum_{\alpha=1}^{N_E} f_i^\alpha \overline{f_j^\alpha} &= \delta_{ij}. \end{aligned} \quad (5.26)$$

If we suppose that the initial state of the environment is given by $\sigma_E(0) = |E\rangle\langle E|$ then some simple algebra shows that for an arbitrary initial state $\rho(0)$ of the system of interest we obtain:

$$\text{Tr}_E \left\{ U_t (\rho(0) \otimes |E\rangle\langle E|) U_t^\dagger \right\} = |\psi_S\rangle\langle\psi_S|$$

with the resulting state vector of the system of interest given by

$$|\psi_S\rangle = \sum_{i=1}^{N_S} \sum_{\beta}^{N_E} f_i^{\beta} \langle \varphi_{\beta}|E\rangle |i\rangle.$$

If we want to write this in terms of a completely positive map, the Kraus operators would be given by

$$W^{\gamma} = |\psi_S\rangle \langle b^{\gamma}|,$$

where

$$|b^{\gamma}\rangle = \sum_{m=1}^{N_S} \overline{g_m^{\gamma}} |m\rangle.$$

The vectors $|b^{\gamma}\rangle$ have some very interesting properties stemming from the restrictions (5.25) and (5.26), in particular it is easy to verify that they satisfy the completeness relation

$$\sum_{\gamma=1}^{N_E} |b^{\gamma}\rangle \langle b^{\gamma}| = \mathbf{1}_S,$$

and the orthogonality relation

$$\langle b^{\alpha}|b^{\beta}\rangle = \delta_{\alpha\beta} \quad \forall \alpha, \beta = 1, \dots, N_E. \quad (5.27)$$

This last property has serious implications for our model. From the entropy considerations in section 5.1 it is easy to see why for the process to work we need $N_E \geq N_S$. However, due to the assumption of a finite Hilbert space of $\dim \{\mathfrak{H}_S\} = N_S$ for the system of interest, we know that any orthonormal set $\{|b^{\gamma}\rangle\}$ of \mathfrak{H}_S can have at most N_S distinct elements. This upper limit together with the orthonormal relation (5.27) implies that the dimension of the Hilbert space of our environment has to be of the same dimension as that of the system, i.e. for our scheme to be consistent we need $N_E = N_S$.

Therefore it seems that we have recovered a set of Kraus operators equivalent to the ones in (5.21) resulting from our original ansatz, but in doing so we have realized that for these operators to result from the unitary evolution of an initially factorized state then the “environment” needs to be of the same dimension as the system of interest.

As an example to better understand the unitary evolution U in (5.24) let us consider the particular situation where $f_i^{\beta} = \delta_{i\beta}$ and $g_m^{\alpha} = \delta_{m\alpha}$ (obviously $N_S = N_E$). In this case one easily sees that

$$U(\rho_S \otimes \sigma_E)U^{\dagger} = \sigma_S \otimes \rho_E.$$

That is, this particular example of U results in a swap operation where the states of the system and the environment are interchanged. Therefore, if the initial state of the environment is pure it is obvious why the state of the system of interest will be purified. Nonetheless, let us stress the fact that this is just one particular example and there exist several other possibilities for U resulting in a purification but not in a perfect state transfer.

Finally, we would like to know if our map (5.21) is the only type of completely positive map that yields a pure state for the system of interest or if there are other options. To this end let us

extend the system of interest so as to introduce an ancillary system described by a Hilbert space \mathfrak{H}_A with trivial dynamics. Now, let us make the obvious remark that if the state $\rho_S = \text{Tr}_A \{\rho_{SA}\}$ ($\rho_{SA} \in \mathfrak{B}(\mathfrak{H}_S \otimes \mathfrak{H}_A)$) is to be pure then the state ρ_{SA} needs to be factorizable, i.e. there can be no entanglement between the original system of interest and the ancilla. If we accept this then we can exploit a powerful result by [Horodecki *et al.* 2003] that says that a completely positive map $(\hat{\Lambda}^{E-B} \otimes \mathbf{1}_A)[\rho_{SA}]$ resulting in a separable state for *any* ρ_{SA} can always be written as

$$\hat{\Lambda}^{E-B} \rho_S(0) = \sum_{\eta} \rho_{\eta} \text{Tr} \{F_{\eta} \rho_S(0)\},$$

where ρ_{η} , for every η , are density matrices belonging to $\mathfrak{B}(\mathfrak{H}_S)$, and the operators F_{η} are positive and obey $\sum_{\eta} F_{\eta} = \mathbf{1}$ if the map is trace-preserving. The superoperator $\hat{\Lambda}^{E-B}$ is called an *entanglement breaking map*.

Therefore, if the map $\hat{\Lambda}^{E-B}$ is to result in a pure state for an arbitrary initial state ρ_S , and since pure states are extremal states, we have that the only option is

$$\begin{aligned} \hat{\Lambda}^{E-B} \rho_S &= \Psi \text{Tr} \left\{ \sum_{\eta} F_{\eta} \rho_S(0) \right\} \\ &= \Psi \text{Tr} \{ \rho_S(0) \} \\ &= \Psi, \end{aligned}$$

where Ψ is the pure state to which *all* states are driven to. This means that any completely positive map that results in a purification for an arbitrary initial state of the system of interest must be of this *degenerate* form where all of the state space is mapped to a unique pure fixed point independently of the initial state.

In conclusion, we have shown that there exists a non-Markovian physical processes that yields a “universal” purifying completely positive map that agrees with our ansatz (5.18). However, our greediness of a CCP for an arbitrary initial state, resulted in the pure state being independent of the initial condition. Also, we have proven that if such a map is the result of the unitary evolution of an uncorrelated initial state of the environment then one can only achieve universal purification of the system of interest if the Hilbert space of the environment, \mathfrak{H}_E , is commensurate with the space \mathfrak{H}_S ; and furthermore the initial state of the environment needs to be *pure*. This actually would seem to be a setback to our objective of producing pure states, since it turns out that in this scheme to produce a pure state we need an environment in a pure state thus defeating our purpose. In the next sections we will study other alternatives.

5.5 Quasi-reversible transformations performed at or near equilibrium (Cooling)

If you were to ask a physicist how one usually prepares a pure state he or she would almost certainly answer that this is achieved either by cooling or by a measurement procedure. Here we want to briefly show in what cases the former is valid, the latter will be analyzed in the next chapter.

If the system of interest is at equilibrium with a heat bath at temperature T , with which it interacts weakly, then the state of the system would be:

$$\rho(\beta) = \frac{1}{Z(\beta)} e^{-\beta H} \quad (5.28)$$

where as usual $\beta = \frac{1}{k_B T}$ and $Z(\beta)$ is the partition function given by

$$Z(\beta) = \text{Tr} \left\{ e^{-\beta H} \right\} \quad (5.29)$$

Then a suitable measure of the purity of the system at temperature T will be

$$\eta[\rho(\beta)] := \text{Tr} \left\{ \rho^2(\beta) \right\} = \frac{Z(2\beta)}{Z^2(\beta)} \quad (5.30)$$

Now let us assume that the spectrum of H is discrete (at least the portion corresponding to the lowest energy levels which will be the only ones contributing at small temperatures). If we denote by g_i the degeneracy of the energy level E_i the partition function is given by

$$Z(x) = \sum_i g_i e^{-x E_i} \quad (5.31)$$

Furthermore let us assume that if we reduce the temperature of the bath then after a suitable relaxation time the system of interest will reach equilibrium at this reduced temperature. Then, as $T \rightarrow 0$ only the ground state is populated and without any loss of generality let $E_0 = 0$ (this is valid if the Hamiltonian is bounded from below, as it should be for any properly behaved system), hence

$$\lim_{T \rightarrow 0} \eta \left[\rho \left(\frac{1}{k_B T} \right) \right] = \frac{1}{g_0} \quad (5.32)$$

Then it is easy to see that if the ground state of the system is not degenerate then a cooling process will purify it. However, if the ground state is degenerate the cooling mechanism, in this description, will not lead to a pure state and we would need to use one of the other methods mentioned in this work to obtain a pure state.

Since the previous seems to be at odds with certain formulations of the third law of thermodynamics some comments are in order. Broadly speaking, systems with degenerate ground states correspond to many-body systems that usually show phase transitions, and hence broken symmetries. It is well known that for these systems (in the thermodynamic limit) the equivalent ground states are isolated by superselection rules impeding the coherent superposition of these states [Huang 1987], thus forbidding the creation of a pure state formed by coherent superpositions of the equivalent ground states. However, in practice, there will usually be a spurious external field that selects a single ground state forcing the system into a pure state at zero temperature. Having said this, it is important to mention that there are examples of thermodynamic systems that near the absolute zero can be found in metastable states with non-zero entropy, e.g. CO_2 , glycerol, and glasses in general (see for example [Stillinger *et al.* 2001] and references therein).

5.6 Dissipation assisted CCP

The previous model of cooling is basically just an example of dissipation (flow of energy to and from the system of interest) resulting in an equilibrium state. However the idea is quite general. Intuitively, if the system of interest possesses a ground state (its bare Hamiltonian has a lower bound, as is the case for most well behaved models) then there is just so much energy it can shed into the environment before it reaches its ground state which, barring degeneracies, is a unique pure state. Conversely if the system of interest can be described by a Hilbert space of finite dimension, and the state corresponding to the maximum eigenvalue of its bare Hamiltonian is unique, then there is only a certain amount of energy it can absorb before saturating and reaching a pure state. (The last statement is only valid up to a certain approximation. If the energy being fed into the system of interest exceeds a certain threshold the finite-dimensional approximation will break down and the system of interest will be taken into the continuum).

Here we would like to present an example that serves as a model (albeit somewhat simplistic) for the previous comments. As well, our example will serve to confirm the conditions of section 5.2, and our ansatz (5.8) for a CCP map in the case of Markovian dynamics.

Our example consists of a two-level system, interacting with an environment, such that its dynamics are governed by a Lindblad equation of the form:

$$\begin{aligned} \frac{d}{dt}\rho(t) = & -\frac{i}{\hbar}[H_S; \rho(t)] + \gamma_{\uparrow}(2\sigma_+\rho(t)\sigma_- - \sigma_-\sigma_+\rho(t) - \rho(t)\sigma_-\sigma_+) \\ & + \gamma_{\downarrow}(2\sigma_-\rho(t)\sigma_+ - \sigma_+\sigma_-\rho(t) - \rho(t)\sigma_+\sigma_-) \end{aligned} \quad (5.33)$$

with $H_S = \frac{1}{2}\hbar\omega_0\sigma_z$. Observe that the completely positive condition implies that the coupling constants γ_{\bullet} , which have dimensions of inverse time (for this equation they can be roughly interpreted as transfer rates between the eigenstates H_S), are such that $\gamma_{\bullet} \geq 0$. The equation is usually called the *quantum optical master equation*; it can be derived from first principles in the Born-Markov approximation (see section 3.1) from the interaction in the optical regime of a two-level atom with a thermal reservoir composed of non-interacting bosons [Breuer & Petruccione 2002]. In this case the coupling constants are given by:

$$\gamma_{\uparrow} = \gamma_0 \bar{n}, \quad (5.34a)$$

$$\gamma_{\downarrow} = \gamma_0 (\bar{n} + 1), \quad (5.34b)$$

where $\gamma_0 = \frac{4\omega_0 \|\vec{d}\|^2}{3\hbar c^3}$ ($\vec{d} = \langle -|\vec{D}|+ \rangle$ is the transition matrix element of the traceless dipole operator \vec{D}), and $\bar{n} = \bar{n}(\omega_o)$ denotes the Planck distribution at the transition frequency ω_o , which reads:

$$\bar{n} = \frac{1}{e^{\beta\hbar\omega_o} - 1}.$$

In this case, we should expect the system of interest to reach equilibrium (which it does, see equation 5.38 below) since the coupling constants (transfer rates) obey the detailed balance condition $\gamma_{\downarrow}/\gamma_{\uparrow} = e^{\beta\hbar\omega_o}$.

Nonetheless, equation (5.33) also arises in phenomenological descriptions of two-level systems exchanging energy with an environment [Alicki 2002]. In particular if $\gamma_{\uparrow} \neq 0$ and $\gamma_{\downarrow} = 0$ the model describes the pumping of energy into the system of interest (without emission), whereas if $\gamma_{\uparrow} = 0$ and $\gamma_{\downarrow} \neq 0$ it can describe spontaneous decay into the vacuum.

The master equation (5.33) is easily solved for $\rho(t)$, however here we will calculate the associated map so as to compare it with the previous results. As in previous section let us define $\rho(t) = \hat{\Lambda}(t) [\rho(0)]$ and rewrite (5.33) in the form of equation (3.24), viz:

$$\begin{aligned} \frac{d}{dt} \hat{\Lambda}(t) = & (-i\hat{\mathcal{L}}_{H_S} + \gamma_{\uparrow} \left(\hat{L}_{\sigma_+} \hat{R}_{\sigma_-} - \frac{1}{2} \hat{R}_{\sigma_+} \hat{R}_{\sigma_-} - \frac{1}{2} \hat{L}_{\sigma_-} \hat{L}_{\sigma_+} \right) + \\ & \gamma_{\downarrow} \left(\hat{L}_{\sigma_-} \hat{R}_{\sigma_+} - \frac{1}{2} \hat{R}_{\sigma_-} \hat{R}_{\sigma_+} - \frac{1}{2} \hat{L}_{\sigma_+} \hat{L}_{\sigma_-} \right)) \hat{\Lambda}(t), \end{aligned} \quad (5.35)$$

with the initial condition $\hat{\Lambda}(0) = \hat{\mathbf{1}}$. Then, in the canonical basis $\{|+\rangle\langle+|, |-\rangle\langle-|, |+\rangle\langle-|, |-\rangle\langle+|\}$ (where $|+\rangle, |-\rangle$ are the eigenvectors of σ_z and the state would be represented by the vector $\vec{\rho} = (\rho_{++}, \rho_{--}, \rho_{+-}, \rho_{-+})^T$) the solution of equation (5.35), denoted by $\hat{\Lambda}^{can-Z}$, would be:

$$\hat{\Lambda}^{can-Z}(t) = \begin{pmatrix} \frac{1}{\gamma_{\uparrow} + \gamma_{\downarrow}} \times (\gamma_{\uparrow} + \gamma_{\downarrow} e^{-2(\gamma_{\uparrow} + \gamma_{\downarrow})t}) & \frac{\gamma_{\uparrow}}{\gamma_{\uparrow} + \gamma_{\downarrow}} \times (1 - e^{-2(\gamma_{\uparrow} + \gamma_{\downarrow})t}) & 0 & 0 \\ \frac{\gamma_{\downarrow}}{\gamma_{\uparrow} + \gamma_{\downarrow}} \times (1 - e^{-2(\gamma_{\uparrow} + \gamma_{\downarrow})t}) & \frac{1}{\gamma_{\uparrow} + \gamma_{\downarrow}} \times (\gamma_{\downarrow} + \gamma_{\uparrow} e^{-2(\gamma_{\uparrow} + \gamma_{\downarrow})t}) & 0 & 0 \\ 0 & 0 & e^{-(\gamma_{\uparrow} + \gamma_{\downarrow})t} \times e^{+i\omega_0 t} & 0 \\ 0 & 0 & 0 & e^{-(\gamma_{\uparrow} + \gamma_{\downarrow})t} \times e^{-i\omega_0 t} \end{pmatrix} \quad (5.36)$$

Notice that this representation is of the form of the one in (5.6), with classicality being defined with respect to the eigenvectors of σ_z . For this partition of the Hilbert space, the map $\hat{\Lambda}$ preserves classicality ($\Lambda_{QC} = 0$). In fact, if there is any initial coherence (specific to this representation) this will decay with a characteristic time of $1/(\gamma_{\uparrow} + \gamma_{\downarrow})$. Also, if we define the diagonal relaxation time as $\tau_{\parallel} = 1/2(\gamma_{\uparrow} + \gamma_{\downarrow})$ and the off-diagonal relaxation time as $\tau_{\perp} = 1/(\gamma_{\uparrow} + \gamma_{\downarrow})$, then it is easy to see that they obey the Bloch relation $\tau_{\perp} \leq 2\tau_{\parallel}$ mentioned at the beginning of section 3.5.

It is also instructive to shift to the Bloch sphere representation where the state is represented as $\vec{\rho} = (1, \langle\sigma_x\rangle, \langle\sigma_y\rangle, \langle\sigma_z\rangle)^T$. For this we can transform the map $\hat{\Lambda}^{can-Z}$ to the basis given by the generators of $SU(2)$ by using the unitary matrix (A.5) described in appendix A. In this representation the map reads:

$$\begin{aligned} \hat{\Lambda}^{SU}(t) &= \hat{U}_{SU-Z} \hat{\Lambda}^{can-Z}(t) \hat{U}_{SU-Z}^{\dagger} \\ &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & e^{-(\gamma_{\uparrow} + \gamma_{\downarrow})t} \cos\{\omega_0 t\} & -e^{-(\gamma_{\uparrow} + \gamma_{\downarrow})t} \sin\{\omega_0 t\} & 0 \\ 0 & e^{-(\gamma_{\uparrow} + \gamma_{\downarrow})t} \sin\{\omega_0 t\} & e^{-(\gamma_{\uparrow} + \gamma_{\downarrow})t} \cos\{\omega_0 t\} & 0 \\ \frac{\gamma_{\uparrow} - \gamma_{\downarrow}}{\gamma_{\uparrow} + \gamma_{\downarrow}} \times (1 - e^{-2(\gamma_{\uparrow} + \gamma_{\downarrow})t}) & 0 & 0 & e^{-2(\gamma_{\uparrow} + \gamma_{\downarrow})t} \end{pmatrix} \end{aligned} \quad (5.37)$$

As expected this expression coincides with the general form given in (3.8).

In the particular case where the environment is in thermal equilibrium, and the coupling constants are given by (5.34), it is easily seen from (5.37) that for times $t \gg \tau_\perp$ any initial state will be driven to one in thermal equilibrium, viz:

$$\begin{aligned} \lim_{t \gg \tau_\perp} \langle \sigma_z \rangle(t) &= \frac{\gamma_\uparrow - \gamma_\downarrow}{\gamma_\uparrow + \gamma_\downarrow} \\ &= \frac{e^{-\beta \hbar \omega_0/2} - e^{\beta \hbar \omega_0/2}}{e^{-\beta \hbar \omega_0/2} + e^{\beta \hbar \omega_0/2}}. \end{aligned} \quad (5.38)$$

However, in the special (non-thermal) cases where $\gamma_\uparrow \gg \gamma_\downarrow$ or $\gamma_\uparrow \ll \gamma_\downarrow$, for times $t \gg \tau_\perp$, dissipation drives the system to the pure states characterized by $\langle \sigma_z \rangle = 1$ or $\langle \sigma_z \rangle = -1$ respectively. Notice that the extreme case $\gamma_\uparrow = 0$ ($\gamma_\uparrow \ll \gamma_\downarrow$) coincides with the thermal case (5.38) in the low temperature limit, $\beta \rightarrow \infty$. However, as expected, the high temperature limit, $\beta \rightarrow 0$, results in $\langle \sigma_z \rangle = 0$ (in this limit, from equation 5.34, we see that $\gamma_\downarrow \simeq \gamma_\uparrow$).

Thus, under certain conditions, the map resulting from (5.33) is capable of resulting in a pure state. However, this state corresponds to a classical extreme state if we define classicality in the σ_z representation. But the choice for the partition with respect to which classicality is defined for this model is rather arbitrary (even more so than in usual decoherence models). In fact, the master equation (5.33) possesses a unique fixed point inside the state space given by (in the σ_z representation):

$$\rho_{fix} = \begin{pmatrix} \frac{\gamma_\uparrow}{\gamma_\uparrow + \gamma_\downarrow} & 0 \\ 0 & \frac{\gamma_\downarrow}{\gamma_\uparrow + \gamma_\downarrow} \end{pmatrix},$$

but its eigenvectors (which are simply $|+\rangle$ and $|-\rangle$), even in the extreme cases $\gamma_\uparrow \gg \gamma_\downarrow$ or $\gamma_\uparrow \ll \gamma_\downarrow$ yielding a pure state, are not conserved. Therefore in our model it is not possible to define a proper pointer basis, in the sense of Zurek, that is not affected by the environment (see section 4.1).

Bearing in mind the previous let us redefine classicality for this example so as it is defined with respect to the partition generated by the projectors $\{|\rightarrow\rangle\langle\rightarrow|, |\leftarrow\rangle\langle\leftarrow|\}$, where $|\rightarrow\rangle$ and $|\leftarrow\rangle$ are the eigenvectors of σ_x . In this case we would be interested in writing the map $\hat{\Lambda}(t)$ in the associated canonical basis $\{|\rightarrow\rangle\langle\rightarrow|, |\leftarrow\rangle\langle\leftarrow|, |\rightarrow\rangle\langle\leftarrow|, |\leftarrow\rangle\langle\rightarrow|\}$. This is easily done, just as in (5.37), by using the unitary matrix (A.4) given in appendix A. Obviously this change in the definition of classicality will result in the map generating coherence in this representation. If we use the notation $\hat{\Lambda}^{can-X}(t) = \hat{U}_{X-Z} \hat{\Lambda}^{can-Z}(t) \hat{U}_{X-Z}^\dagger$, it is easy to see that the block matrix $(\hat{\Lambda}^{can-X})_{QC}$ will have all of its components different from zero. Let us focus on the long time regime where $t \gg \tau_\perp$. In this limit the map is given by

$$\lim_{t \gg \tau_\perp} \hat{\Lambda}^{can-X}(t) = \frac{1}{2} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ \frac{\gamma_\uparrow - \gamma_\downarrow}{\gamma_\uparrow + \gamma_\downarrow} & \frac{\gamma_\uparrow - \gamma_\downarrow}{\gamma_\uparrow + \gamma_\downarrow} & 0 & 0 \\ \frac{\gamma_\uparrow - \gamma_\downarrow}{\gamma_\uparrow + \gamma_\downarrow} & \frac{\gamma_\uparrow - \gamma_\downarrow}{\gamma_\uparrow + \gamma_\downarrow} & 0 & 0 \end{pmatrix}. \quad (5.39)$$

The point of this expression is that it verifies the trivial result that since the dynamics given by (5.33) result in the long time regime in a state diagonal in the σ_z representation then in the σ_x

representation the state will be non-diagonal, hence $\left(\hat{\Lambda}^{can-X}\right)_{QC} \neq 0$. As well, in the extreme cases $\gamma_{\uparrow} \gg \gamma_{\downarrow}$ or $\gamma_{\uparrow} \ll \gamma_{\downarrow}$ yielding pure states, it is easy to see that (5.39) satisfies our ansatz (5.8) for the general structure of a map resulting in a pure state. For example in the case that $\gamma_{\uparrow} \ll \gamma_{\downarrow}$ we have that $\hat{\Lambda}^{can-X}(t)$ is of the form $\left(\hat{\Lambda}^{FixP}\right)_{ij}^{mn} = \alpha_i \bar{\alpha}_j \delta_{mn}$ with $\alpha_{\rightarrow} = 1/\sqrt{2}$ and $\alpha_{\leftarrow} = -1/\sqrt{2}$.

Finally we would like to mention that, although we have seen that the master equation (5.33) can, under certain conditions, result in a purifying map consistent with our ansatz (5.8), we have not been able to study the inverse problem. That is, we have not been able to use our ansatz to deduce any useful conditions for the form of a Lindblad equation producing a pure state as we did in the non-Markovian case. Nonetheless, some obvious conditions the master equations should obey to produce a map of the type $\hat{\Lambda}^{FixP}$ are that it should, in some suitable time region, say $t \gg \tau_{CCP}$, possess a unique pure fixed point. This is apart from the basic requirement that the form of the Lindblad equation should allow for the possibility of a decrease of entropy (as we will see in section 6.4 this is not always the case).

5.7 A case study of inverse maps: generalized depolarizing channels

In this section we will analyse the generalized depolarizing channel \hat{D}_{κ} defined as:

$$\hat{D}_{\kappa}\rho = \kappa\rho + (1 - \kappa) \frac{\mathbf{1}}{n}, \quad (5.40)$$

with $\kappa \in [-\frac{1}{n^2-1}, \infty)$, and n is the (finite-)dimension of the Hilbert space of the system of interest whose states are described by ρ . Usually the depolarizing channel is defined with $\kappa \in [0, 1]$, although complete positivity only demands $-(n^2 - 1)^{-1} \leq \kappa \leq 1$ [King 2002]. However, for reasons that will become apparent below, we have chosen to define it with a more general range of positive values for the parameter κ .

The depolarizing map, with $\kappa \in [0, 1]$, is widely used in the quantum information community to model the effect of noise in quantum computers [Nielsen & Chuang 2000]. Thus, there has been some effort devoted to finding techniques to reverse the effect of this map so as to regenerate the original state. However, these attempts assume that the map is not invertible (reversible) and therefore they need to use techniques that utilize multiple copies of the system of interest and then only obtain a limited rate of success [Cirac *et al.* 1999] [Keyl & Werner 2001].

Nonetheless, it is not exactly true that the depolarizing channel is not invertible. In fact it is easily verified that its inverse is just another depolarizing channel, but with a parameter $1/\kappa$, viz:

$$\begin{aligned} \hat{D}_{\frac{1}{\kappa}} \hat{D}_{\kappa} \rho &= \frac{1}{\kappa} \left(\kappa \rho + (1 - \kappa) \frac{\mathbf{1}}{n} \right) + \left(1 - \frac{1}{\kappa} \right) \frac{\mathbf{1}}{n} \\ &= \rho. \end{aligned} \quad (5.41)$$

That is

$$\hat{D}_{\kappa}^{-1} = \hat{D}_{\frac{1}{\kappa}}.$$

The problem is that in general the depolarizing channel supposes that $0 \leq \kappa \leq 1$, which is interpreted as a mixing with probability κ of the original state with a maximally mixed state. Hence the physical interpretation of a “depolarizing” channel with a control parameter $\kappa > 1$ is far from obvious. Yet, this is just a technicality since, if we accept that any completely positive map is physically realizable [Kraus 1983] then we would have a similar interpretational difficulty when $-(n^2 - 1)^{-1} \leq \kappa < 0$ which still corresponds to a completely positive map.

Another difficulty with our inverse map is that the domain of definition of \hat{D}_κ , with $\kappa > 1$, is restricted in the sense that it does not coincide with the whole of the state space $S(\mathfrak{A}) \subset \mathfrak{B}(\mathfrak{H})$ if it is to map every state in its domain to another state. However, as we saw in section 3.5, there are situations where it does not make sense to apply a map to every state in $S(\mathfrak{A})$ (that is, there are processes that are only physical if applied to a limited set of initial states). In fact, even if we limit ourselves to $\kappa \in [0, 1]$, the map is somewhat restricted in the sense that it is only convex and not strictly linear. The relationship $\hat{D}_\kappa(aA + bB) = a\hat{D}_\kappa A + b\hat{D}_\kappa B$ only holds if $a + b = 1$.

Therefore, bearing this in mind, we will investigate what is the subset of states $\tilde{A}_\kappa \subset S(\mathfrak{A})$, which, following the convention in section 3.5, we will refer to as the positivity domain of \hat{D}_κ , whose image is contained in $S(\mathfrak{A})$ under the action of our generalized depolarizing channel when $\kappa > 1$. Notice, that because of (5.41) we are assured that \tilde{A}_κ is non-empty; at the very least it will contain all the states that result from $\hat{D}_{\frac{1}{\kappa}}\rho$ for every $\rho \in S(\mathfrak{A})$ and the state $\frac{1}{n}$ which is a fixed point of the map for any value κ .

To establish a necessary condition (but sadly not sufficient for dimensions $n \geq 3$) for $\rho \in \tilde{A}$ we will use some geometrical arguments that exploit the fact that $\frac{1}{n}$ can be thought as a centre of $S(\mathfrak{A})$ if we use the trace norm metric defined as:

$$d(A, B) := \|A - B\|_1 \quad (5.42)$$

where $A, B \in \mathfrak{B}(\mathfrak{H})$, and the trace norm is defined as

$$\|A\|_1 := \text{Tr} \left\{ \sqrt{A^\dagger A} \right\} \equiv \text{Tr} \{|A|\}. \quad (5.43)$$

(Since we are implicitly working in a finite dimensional Hilbert space we do not have to worry about the convergence of the trace norm).

For pure states represented by one dimensional projectors Ψ_1 and Ψ_2 ($\Psi_i = |\psi_i\rangle\langle\psi_i|$), this distance can be calculated as

$$\|\Psi_1 - \Psi_2\|_1 = 2\sqrt{1 - \text{Tr} \{\Psi_1 \Psi_2\}}, \quad (5.44)$$

(this last result also holds in the infinite dimensional case [Roberts & Roepstorff 1969, lemma 4.6]) which is determined by the usual transition probability

$$\text{Tr} \{\Psi_1 \Psi_2\} = |\langle\psi_1|\psi_2\rangle|^2.$$

The reason why we refer to $\frac{1}{n}$ as a centre of $S(\mathfrak{A})$ (apart from the fact that it belongs to any classical set \tilde{C}) is because it is equidistant from all the extremal states of $S(\mathfrak{A})$, viz:

$$d\left(\Psi, \frac{1}{n}\right) = 2\left(1 - \frac{1}{n}\right), \quad \forall \Psi \in \partial S(\mathfrak{A}).$$

This statement can be easily verified and we have included a proof of it in appendix B (we have also included in this appendix some other simple results that are used below and that lend further weight to the naming of the pure states as extremes). Since this last value will play a special rôle in what follows let us denote it as

$$m_n^{sat} = 2 \left(1 - \frac{1}{n} \right).$$

Also for convenience let us use the notation:

$$m_B = d \left(B, \frac{\mathbf{1}}{n} \right), \quad \forall B \in \mathfrak{B}(\mathfrak{H}). \quad (5.45)$$

Using the results in appendix B we have that any valid state needs to satisfy:

$$0 \leq m_\rho \leq m_n^{sat}, \quad \forall \rho \in S(\mathfrak{A}). \quad (5.46)$$

Where the equality on the rhs only holds if ρ is pure, and the equality on the lhs if $\rho = \frac{\mathbf{1}}{n}$.

Now notice that the depolarizing channel has a simple scaling relation with our distance m_B , viz:

$$\begin{aligned} d \left(\hat{D}_\kappa \rho, \frac{\mathbf{1}}{n} \right) &= \text{Tr} \left\{ \sqrt{\left(\kappa \rho - \kappa \frac{\mathbf{1}}{n} \right)^2} \right\} \\ &= |\kappa| d \left(\rho, \frac{\mathbf{1}}{n} \right). \end{aligned}$$

Therefore we have that

$$m_{\hat{D}_\kappa \rho} = |\kappa| m_\rho. \quad (5.47)$$

This last relation, together with (5.46), gives us a necessary (but not sufficient) criterion for the possible range of values the parameter κ can have if the the action of the depolarizing channel is to result in a state. Namely if $\hat{D}_\kappa \rho$ is to belong to $S(\mathfrak{A})$ then κ needs to satisfy the condition

$$|\kappa| \leq \frac{m_n^{sat}}{m_\rho}.$$

Thus, for a fixed value of $\kappa > 1$, we could be tempted to define the positivity domain of the depolarizing map \hat{D}_κ as:

$$\tilde{A}'_\kappa = \left\{ \rho \in S(\mathfrak{A}) \mid m_\rho \leq \frac{m_n^{sat}}{\kappa} \right\}. \quad (5.48)$$

It is obvious that if $(\hat{D}_\kappa \rho) \in S(\mathfrak{A})$ then $\rho \in \tilde{A}'_\kappa$. However, as we will see below, the converse is not true for $n \geq 3$; i.e. *not* every $\rho \in \tilde{A}'_\kappa$ will be mapped by \hat{D}_κ into $S(\mathfrak{A})$ when $n \geq 3$.

To see why $\rho \in \tilde{A}'_\kappa$ is only a necessary, but not sufficient, condition notice that the scaling relation (5.47) would seem to suggest that there always exists a generalized “depolarizing” channel that could purify *any* state for every dimension n (except for $\frac{\mathbf{1}}{n}$ which is a fixed point). That is, we could naïvely be driven to write for every state with $m_\rho \neq 0$

$$\hat{D}_{m_n^{sat}/m_\rho} \rho = \Psi. \quad (5.49)$$

However, this is obviously wrong (it would be too good to be true if we could purify any state like this). To see this notice that if (5.49) were true then some trivial algebra would give us the relation

$$m_\rho = 2\sqrt{\left(1 - \frac{1}{n}\right) \left(\text{Tr}\{\rho^2\} - \frac{1}{n}\right)}. \quad (5.50)$$

This relation can be easily verified to be true for $n = 2$. However for $n = 3$ consider the following counterexample, suppose that the state is given by the diagonal matrix $\rho = \text{diag}\left\{\frac{3}{6}, \frac{2}{6}, \frac{1}{6}\right\}$, which yields $m_\rho = 1/3$ and $\text{Tr}\{\rho^2\} = 7/18$. These values do not comply with the relation (5.50). Nonetheless, the relationship will hold for any n if ρ is the result of the action of a depolarizing channel on a pure state.

It is actually quite simple to understand why the criterion $\rho \in \tilde{A}'_\kappa$ does not work for $n \geq 3$. The problem lies in the fact that not every $\rho \in S(\mathfrak{A})$ satisfies (5.49). If this were true then we would have that every single state in $S(\mathfrak{A})$ could be written as $\hat{D}_\kappa \Psi$, for some suitable pure state Ψ and $\kappa = m_\rho/m_n^{\text{sat}}$. But a simple count of the parameters needed to describe the system shows this to be incorrect in the general case. The number of real parameters describing a general mixed state is $n^2 - 1$, and the number of real parameters for a pure state is $2(n - 1)$. Thus, a state susceptible to being written as $\hat{D}_\kappa \Psi$ can only encode $2n - 1$ real parameters. Therefore, for $n \geq 3$ we cannot generate all the states in $S(\mathfrak{A})$ by the action of a depolarizing map on the extreme states. This leads us to conjecture that the (true) positivity domain for \hat{D}_κ , when $\kappa > 1$, is the set

$$\tilde{A}_\kappa = \left\{ \rho' \in S(\mathfrak{A}) \mid \rho' = \hat{D}_{1/\kappa} \rho, \forall \rho \in S(\mathfrak{A}) \right\}. \quad (5.51)$$

Trivially we have that $\tilde{A}_\kappa \subseteq \tilde{A}'_\kappa$. In fact, this is quite general and our conjecture provides us with a lower bound on the possible positivity domain (if it does not actually coincide with (5.51)). Notice as well that the size of \tilde{A}_κ relative to $S(\mathfrak{A})$ decreases with increasing n .

These results are readily visualized in the case of a two-dimensional system (where \tilde{A}'_κ is the correct positivity domain) in the Bloch sphere representation. The action of the depolarizing channel on the Bloch vector is simply a rescaling of its length, viz:

$$(\langle \sigma_x \rangle, \langle \sigma_y \rangle, \langle \sigma_z \rangle) \xrightarrow{\hat{D}_\kappa} \kappa (\langle \sigma_x \rangle, \langle \sigma_y \rangle, \langle \sigma_z \rangle).$$

Therefore it is easy to understand why, if $n = 2$, \tilde{A}'_κ is the correct positivity domain. If $\kappa > 1$, then the map can only act on states contained in the contracted sphere of radius $1/\kappa$; if not, the dilation generated by the depolarizing channel would push some of the states outside the boundary of valid states defined by the sphere of radius $m_2^{\text{sat}} = 1$. However, for $n \geq 3$ and an equivalent basis (e.g. the one formed by the generators of $\text{SU}(n)$), this picture ceases to be valid since not all inner states are formed by a uniform contraction of the extremes.

The interesting point about $\tilde{A}_\kappa \neq \tilde{A}'_\kappa$ for $n \geq 3$ is that, although we have shown that $\frac{1}{n}$ is equidistant from the extreme states, it is not possible to connect every state ρ with the centre $\frac{1}{n}$ and some extreme state with a “straight line” generated by the depolarizing map (which satisfies the scaling relation 5.47). If this were possible we would have a geodesic type condition of the form

$$d\left(\frac{1}{n}, \rho\right) + d\left(\rho, \hat{D}_{m_n^{\text{sat}}/m_\rho} \rho\right) = d\left(\frac{1}{n}, \hat{D}_{m_n^{\text{sat}}/m_\rho} \rho\right) = m_n^{\text{sat}},$$

which is not true. Nonetheless this does not mean that we are certain that there does not exist an extreme state Ψ that minimizes the triangle equality in the sense that $d(\frac{1}{n}, \rho) + d(\rho, \Psi) = d(\frac{1}{n}, \Psi)$ for every ρ . Actually, if we accepted the statement [Thirring 1981 vol. 3, pg. 23]: “A theorem of Krein and Milman says that our naïve idea of convex, compact sets is valid for states; there must exist extremal points and their convex combinations are dense in the space of states.” Then we could be tempted to believe that such a pure state does indeed exist for every ρ . (The argument would involve the use of C^* -algebras² and the fact that the state space is compact in the operator norm topology, however we will not pursue this discussion any further).

To summarize, we have shown that the inverse of the depolarizing channel is properly defined over a non-empty subset of $S(\mathfrak{A})$ in the sense that its action will result in another state. In particular for a two-level system the positivity domain is given by \tilde{A}'_κ defined in (5.48). In the general case, $n \geq 3$, a lower bound for the positivity domain is given by \tilde{A}_κ in (5.51). Nonetheless, although we have seen that in the case where there are initial correlations between the system of interest and the environment the presence of restricted domains is common (see section 3.5), we are still not sure if the map \hat{D}_κ , with $\kappa > 1$, is anything more than a mathematical curiosity or if it is physically realizable for a suitable subset of states.

²For an accesible introduction to the topic of C^* -algebras we recommend the article [Landsman 1998].

Chapter 6

Purifications and Measurements

Following the approach of the previous chapter we will switch from searching for ways to produce Q-states in general, and instead we will only concentrate on how one can obtain a pure state from measurements of the state of the system of interest.

6.1 Ideal measurements and croppings

If we were to again ask a physicist how can one prepare a pure state, he or she would almost certainly answer that this is achieved through measurements (the other common answer would be cooling -which was considered in the preceding chapter). However, not all measurements will result in such a purification and, for completeness, in this section we will make a brief study of the (rather trivial) conditions for measurements (as described in section 2.1) to result in a pure state.

Let us consider first the case of selective projective measurements described by the collection of projectors $\{P_\mu\}_{\mu=1}^m$ ($m \leq \dim \{\mathfrak{H}\}$) forming a partition of the Hilbert space \mathfrak{H} , i.e. $\sum_{\mu=1}^m P_\mu = \mathbf{1}$ and $P_\mu P_\nu = \delta_{\mu\nu} P_\mu$. In the case that $m = \dim \{\mathfrak{H}\}$, the projectors will be one dimensional (following the convention in section 1.5.1 we will call this a fine-grained partition) and can be written as $P_\mu = |\mu\rangle\langle\mu|$. For this situation it is trivial to see that upon measurement an arbitrary state will be transformed into a pure state. Namely, if the outcome μ is registered, the state after the measurement will be:

$$\rho \rightarrow |\mu\rangle\langle\mu|, \quad \forall \rho.$$

Yet, if the partition is coarse grained, i.e. $m < \dim \{\mathfrak{H}\}$, it is also rather easy to see that if the outcome does not correspond to one associated with a one-dimensional projector then the resulting state will in general not be pure unless it was pure before the measurement. To see this suppose that the outcome corresponds to the projector $P_\mu = |\mu\rangle\langle\mu| \otimes \mathbf{1}$, which is obviously not one-dimensional. Furthermore, suppose that the state before the measurement is the mixed state $|\mu\rangle\langle\mu| \otimes \rho$. Then the state immediately after the measurement will be $|\mu\rangle\langle\mu| \otimes \rho$ which is not pure by definition (however, as we will see in section 6.3, this situation can change in the quantum Zeno limit).

The same comment applies to POVMs. If the state before the measurement is a pure state,

$\rho = |\psi\rangle\langle\psi|$, then a selective POVM will always result in another pure state described by

$$|\psi\rangle \rightarrow \frac{1}{\sqrt{\langle\psi|M_\mu^\dagger M_\mu|\psi\rangle}} M_\mu |\psi\rangle.$$

In the case that the initial state is not a pure state, a selective measurement will, in general, not lead to a pure state as an outcome.

From its definition in equation (2.4) it is also easy to see that non-selective measurements will always yield mixed states independently of whether the initial state was pure or not. The only exception in which it could result in a pure state is if the non-selective measurement is performed on a pure state and the measurement operators satisfied the special condition $M_n^\dagger M_m = \delta_{mn} \mathbf{1}$. However, this would be a completely useless type of measurement. From (2.3) we see this would mean that we only have a single measurement operator, which would be the identity.

Therefore, within this standard approach to measurements in Quantum Mechanics, it would seem that the only way to obtain with certainty a pure state is if a non-degenerate observable is measured and if the experimentalist has the exquisite ability to detect all of the fine-grained outcome possibilities. However this is not necessarily exactly true. It is our impression that in practice it is often the case that the experimentalist can, at a first instance, “crop” the ensemble so as to have states only in a certain region where he has access to fine-grained measurements which would then yield pure states after measurement (if this were not possible, at least for some realizations, it would be questionable, or at the very least speculative, to even speak of the existence of these pure states). Nonetheless, even in this scenario, there is always the need for fine-grained measurements at some stage of the process to obtain pure states through a measurement scheme.

6.2 Mathematical “purification” and pre-measurements

There exists a common technique used in quantum computation and quantum information which is usually referred to as (mathematical) “purification” [Nielsen & Chuang 2000]. However, what is meant by this “purification” is somewhat different from the use we have given to this word in this thesis. To distinguish these two meanings whenever referring to this alternative mathematical “purification” we will always enclose it in quotation marks.

What is usually meant by this “purification” is that given a mixed state ρ_S it is always possible to introduce an auxiliary system A and define a pure state, $|\Phi^{SA}\rangle$, of the composite system, such that $\text{Tr}_A \{|\Phi^{SA}\rangle\langle\Phi^{SA}|\} = \rho_S$. The construction of this mathematical “purification” is quite simple. Suppose that ρ_S has the orthonormal decomposition $\rho_S = \sum_i \lambda_i |\lambda_i^S\rangle\langle\lambda_i^S|$. To “purify” S introduce an auxiliary system A with the same state space, and an orthonormal basis $\{|i^A\rangle\}_i$, then define the composite pure state as

$$|\Phi_{SA}\rangle := \sum_i \sqrt{\lambda_i} |\lambda_i^S\rangle |i^A\rangle. \quad (6.1)$$

It is easy to see that, since $\langle i^A | j^A \rangle = \delta_{ij}$, after the elimination of the A -variables this construction will always yield the state ρ_S .

The sense in which this (mathematical) “purification” differs from the general usage of the purification concept in this thesis is clear. The mathematical “purification” involves a pure state of the system of interest *and* the auxiliary system (the system of interest remains mixed) whereas in general our objective has been to obtain a pure state of the system of interest alone. Furthermore the “purification” procedure is usually considered to be only a mathematical tool without a direct physical significance [Nielsen & Chuang 2000].

It is worth noting that the state $|\Phi_{SA}\rangle$ looks very similar to the premeasurement state resulting from the ideal/strong von Neumann interaction mentioned in section 2.1. However one should not be misled by this to suppose that the state is that “easy” to realize physically (supposing that strong measurements were easy to perform, which in practice they are not). If there actually existed an interaction Hamiltonian resulting in a unitary transformation such that $U|\lambda_i^S\rangle|0^A\rangle = |\lambda_i^S\rangle|i^A\rangle$, for some reference state $|0^A\rangle$ of the auxiliary system A , the action of this transformation would yield $U(\rho_S \otimes |0^A\rangle\langle 0^A|)U^\dagger = \sum_i \lambda_i |\lambda_i\rangle\langle \lambda_i| \otimes |i^A\rangle\langle i^A|$ which obviously does not coincide with $|\Phi_{SA}\rangle$ and is not even a pure state.

Recently [Bassi & Ghirardi 2003] have claimed to provide a “physically precise procedure” to achieve this “purification”. We do not believe their claim to be accurate. Although they show that the above “purification” allows the realisation of any statistical ensemble $\{p_i, |\psi_i\rangle_S \langle \psi_i|\}$ represented by the given density matrix ρ_S (which in itself seems somewhat trivial given the results in [Hughston *et al.* 1993] and [Nielsen 2000]), their physical procedure depends on the preparation of a pure state of the form of $|\Phi_{SA}\rangle$ in (6.1). In their own words: “if we can implement our ‘von Neumann-like ideal interaction scheme’ we can perform the desired purification”. However it is our belief that the crux behind the problem of a physical realization of the mathematical “purification” is similar to our objective of finding a procedure to produce pure states from mixed states. The state $|\Phi_{SA}\rangle$ cannot result from a unitary transformation on the SA system alone (which are the only transformations considered in [Bassi & Ghirardi 2003]) unless the initial state of the composite system was pure to begin with, in which case the physical realization is almost trivial and only requires the implementation of a strong measurement.

6.3 Purification through Zeno-Like Measurements

In this section we will briefly review some results obtained by [Nakazato *et al.* 2003] which touch upon the subject of this thesis and which we will study in a modified setting in the next section. Their main result says that under special conditions a series of frequent projective and *selective* measurements performed only on the system of interest, say A , will drive another system, B , interacting with it, to a pure state.

They start by considering two interacting systems, whose dynamics in between measurements is governed by a Hamiltonian of the form

$$H = H_A + H_B + H_{int}, \quad (6.2)$$

where $H_{A(B)}$ stands for the free Hamiltonian of system $A(B)$ and H_{int} for an interaction between them. They then suppose an uncorrelated initial condition where the system A is in a pure state, i.e. the initial state of the composite system is

$$\rho(0) = |\phi\rangle\langle\phi| \otimes \rho_B(0). \quad (6.3)$$

The measurements performed, N times, only on A , at intervals τ , are represented by the projector

$$P = |\phi\rangle\langle\phi| \otimes \mathbf{1}. \quad (6.4)$$

All their results depend on the properties of the operator

$$V_\phi(\tau) = \langle\phi|e^{-iH\tau}|\phi\rangle \quad (6.5)$$

which only acts on the Hilbert space of system B . They assume that this Hamiltonian is such that the operator $V_\phi(\tau)$ has a discrete spectrum and can be expanded in terms of its right- and left-eigenvectors, respectively $|u_n\rangle$ and $\langle v_n|$, as

$$V_\phi(\tau) = \sum_n \lambda_n |u_n\rangle\langle v_n|, \quad (6.6)$$

where λ_n are its eigenvalues.

Their main result is that in the limit $N \rightarrow \infty$ and $\tau \rightarrow 0$, keeping $N\tau = t$ (which corresponds to the *quantum Zeno* limit [Misra & Sudarshan 1977]¹), the system B is driven to a pure state whenever the maximum eigenvalue of V_ϕ (in terms of absolute values,) λ_{\max} , is unique. In fact under these conditions, independent of its initial state, B is driven to

$$\rho_B^{(\tau)}(N) \xrightarrow{N \rightarrow \infty} \frac{|u_{\max}\rangle\langle u_{\max}|}{\langle u_{\max}|u_{\max}\rangle}, \quad (6.7)$$

with a success probability given by

$$p_{\text{succes}}^{(\tau)}(N) \xrightarrow{N \rightarrow \infty} |\lambda_{\max}|^{2N} \langle u_{\max}|u_{\max}\rangle \langle v_{\max}|\rho_B(0)|v_{\max}\rangle. \quad (6.8)$$

It is exactly this purification which we are interested in. In the next section we will study whether this result is still valid in the case of non-selective measurements without collapse.

6.4 Non-selective continuous monitoring

In this section we would like to study whether one could use a purification technique similar to the one previously presented for selective measurements, but for non-selective measurements.

6.4.1 Double commutator master equation and QZE

Consider the following Markovian master equation, which corresponds to the Lindblad equation with a single Hermitian generator $M = M^\dagger$,

$$\frac{d}{dt}\rho = -i[H_S, \rho] - \frac{\gamma}{2}[M, [M, \rho]]. \quad (6.9)$$

Such a double commutator master equation is characteristic of a relaxation process [Kosloff *et al.* 1997], it can be derived from microscopic principles under the assumption of a singular coupling with the (Markovian) environment [Spohn 1980], and it is also typical of a quantum system coupled

¹A report of an experimental realisation of this effect can be found in [Itano *et al.* 1990].

to a stochastic process. In fact, if one supposes that the dynamics of S are governed by a Hamiltonian with a stochastic noise term of the form

$$H'_S = H_S + \eta(t) \sqrt{\gamma} M, \quad (6.10)$$

where $\eta(t)$ corresponds to “white” noise characterized by

$$\langle \eta(t) \rangle = 0, \quad \langle \eta(t) \eta(t') \rangle = c \delta(t - t'), \quad (6.11)$$

then, by averaging over the noise realizations (and taking care of including the Itô correction terms), one can obtain the master equation (6.9) [Pascasio 2004].

However, the master equation (6.9) also appears in the context of quantum measurement theory (see for example [Braginsky & Khalili 1992]). In appendix C we present a derivation of this master equation when one considers the case where the system of interest, described by ρ , interacts continuously with a series of quantum probes measuring (in the sense of von Neumann presented in section 2.1) the observable M of the system of interest. In this context γ is proportional to the accuracy of the measurements, its value regulates whether the measurements are strong or weak in the sense of section 2.2. In fact, in the literature it is claimed that, for large values of γ (strong measurements), this master equation serves to model the equivalent of the *quantum Zeno effect* [Misra & Sudarshan 1977] in the case of *non-selective* measurements [Braginsky & Khalili 1992] [Breuer & Petruccione 2002]. This master equation can also arise in some descriptions of the measurement process in alternative theories/interpretations of quantum mechanics [GRW 1986] [Gisin & Percival 1992] [Pearle 1993] [Adler 2004]. We strongly urge the reader to consult appendix C to see in what sense we believe the double commutator master equation can approximately be thought of as representing a continuous non-selective measurement within the standard Copenhagen interpretation.

The equivalence between the stochastic Hamiltonian and the continuous monitoring character of our master equation is not surprising since the assumptions that lead us to (6.9), described in appendix C, basically imply that the fluctuations in the probe variables have delta-function correlations.

To better understand the master equation (6.9) let us first study a simple example. Namely, let us analyse the equation

$$\frac{d}{dt} \rho_S = -i [H_S, \rho_S] - \frac{\gamma}{2} [\sigma_x, [\sigma_x, \rho_S]], \quad (6.12)$$

with $H_S = \frac{\omega}{2} \sigma_z$. If the interpretation introduced in the previous paragraphs is correct, in principle this example could be interpreted as the dynamics obeyed by a spin- $\frac{1}{2}$ particle during a series of continuous non-selective measurements of its x -component.

Using the same techniques used in section 5.6, the dynamical map $\hat{\Lambda}(t)$ resulting from equation (6.12) is given, in the Bloch sphere representation ($\vec{\rho}(t) = \hat{\Lambda}_t \vec{\rho}(0)$, and $\vec{\rho} = (1, \langle \sigma_x \rangle, \langle \sigma_y \rangle, \langle \sigma_z \rangle)^T$), by:

$$\hat{\Lambda}(t) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & e^{-\gamma t} (\cosh \{\Omega t\} + \frac{\gamma}{\Omega} \sinh \{\Omega t\}) & -\frac{\omega}{\Omega} e^{-\gamma t} \cosh \{\Omega t\} & 0 \\ 0 & \frac{\omega}{\Omega} e^{-\gamma t} \cosh \{\Omega t\} & e^{-\gamma t} (\cosh \{\Omega t\} - \frac{\gamma}{\Omega} \sinh \{\Omega t\}) & 0 \\ 0 & 0 & 0 & e^{-2\gamma t} \end{pmatrix},$$

where $\Omega = \sqrt{\gamma^2 - \omega^2}$. In the case that $\gamma < \omega$, it is easy to see that when $\langle \sigma_x \rangle(0) \neq 0$ and/or $\langle \sigma_y \rangle(0) \neq 0$, the dynamics will consist of damped oscillations and, independent of the initial state, the system of interest will be driven to the maximally mixed state $\frac{1}{2}$ (if $\langle \sigma_x \rangle(0) = 0$, $\langle \sigma_y \rangle(0) = 0$, and $\langle \sigma_z \rangle(0) \neq 0$ the system will be driven to the maximally mixed state without any oscillations). In the case of sufficiently small γ , which would correspond to the case of weak measurements, the damping of the oscillation will be negligible. However, if $\gamma \geq \omega$ there will not be any oscillations.

Let us focus in the extreme case when $\gamma \gg \omega$; in this limit the dynamical map becomes:

$$\lim_{\gamma \gg \omega} \hat{\Lambda}(t) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & e^{-2\gamma t} & 0 \\ 0 & 0 & 0 & e^{-2\gamma t} \end{pmatrix}.$$

This is the limit that is usually interpreted as corresponding to the quantum Zeno effect in the case of non-selective measurements. The initial $\langle \sigma_x \rangle(0)$ component will be conserved for all times while any component off the x direction will be quickly damped out. Thus, there is a freezing of the dynamics (at least for times $t > 1/\gamma$). Nonetheless, although this case corresponds to strong measurements, since they are non-selective, there is no purification of the state (in accordance with our discussion in section 6.1).

This freezing of the dynamics can be easily generalized to higher dimensional systems. If γ is sufficiently large compared to any term in the bare Hamiltonian H_S then the master equation (6.9) can be approximated as

$$\frac{d}{dt} \rho_S \simeq -\frac{\gamma}{2} [M, [M, \rho_S]]. \quad (6.13)$$

If the initial state $\rho(0)$ is an eigenstate of M , or simply if it is such that $[M, \rho(0)] = 0$, then it will remain stationary. All other states will suffer some sort of damping, but the quantity $\langle M \rangle_{\rho(0)}$ will always be conserved for any initial state.

6.4.2 Is there purification for the non-selective QZE?

Given the previous, it is natural to ask whether we could use a technique similar to the one presented in section 6.3, and due to [Nakazato *et al.* 2003], to obtain some sort of purification in the quantum Zeno limit of non-selective measurements described by equation (6.9). Namely, the question we want to address is: If we were to consider a system of interest composed of two subsystems, say A and B (i.e. $\mathfrak{H}_S = \mathfrak{H}_A \otimes \mathfrak{H}_B$); is it possible that the continuous non-selective measurement of a property exclusive to one of the subsystems of interest (as described by equation 6.9), say $M_A \otimes \mathbf{1}_B$, will drive the other subsystem of interest (B) to a pure state while preserving the purity of the first subsystem (A)? Namely we would like to see whether the master equation

$$\frac{d}{dt} \rho_{AB} = -i[H_{AB}, \rho_{AB}] - \frac{\gamma}{2} [M_A \otimes \mathbf{1}_B, [M_A \otimes \mathbf{1}_B, \rho_{AB}]], \quad (6.14)$$

for some particular initial state $\rho_{AB}(0) = \Psi_A \otimes \rho_B \in \mathfrak{B}(\mathfrak{H}_A \otimes \mathfrak{H}_B)$ and Hamiltonian $H_{AB} = H_A + H_B + H_{int}$, could result in the purification of $\rho_B(t) = \text{Tr}_A \{\rho_S(t)\}$ while preserving the

pure state Ψ_A . If this were true we would obtain a pure state for the composite system AB (which is the claim of [Nakazato *et al.* 2003] in the case of selective measurements).

To answer this question let us make a small historical parenthesis. It is worth noticing that the origins of the description of open system dynamics lie in attempts to understand the approach to equilibrium. Therefore a lot of effort has been devoted to study the relationship between master equations and entropy. The problem is complex and there are very few general results. However, an exception to this is the master equation (6.9). In fact, it can be proved that the master equation ($V_j = V_j^\dagger$ for every j)

$$\frac{d}{dt}\rho(t) = -i[H + V(t), \rho(t)] - \frac{1}{2} \sum_j [V_j, [V_j, \rho(t)]] \quad (6.15)$$

satisfies the H-theorem² [Alicki 2002] [Lidar *et al.* 2004]. That is, for any of the solutions of (6.15) we have

$$S_{vN}[\rho(t)] \geq S_{vN}[\rho(s)] \quad \forall t \geq s \geq 0, \quad (6.16)$$

where $S_{vN}[\rho] = -\text{Tr}\{\rho \ln \rho\}$ is the von Neumann entropy.

Equation (6.16) provides the answer to our question. The proposal in [Nakazato *et al.* 2003], for selective measurements, assumes that at $t = 0$ the state of the composite system of interest is strictly a mixed state and of the form $\rho_{AB}(0) = |\psi\rangle\langle\psi| \otimes \rho_B$ which implies $S_{vN}[\rho_{AB}(0)] = S_{vN}[\rho_B(0)] > 0$. However, if we followed Nakazato's ideas, and used this initial condition in equation (6.14) with $M_A = |\psi\rangle\langle\psi|$ and the system were purified after a sufficiently long time t then we would have $\rho_{AB}(t) = |\psi\rangle\langle\psi|_A \otimes |\phi\rangle\langle\phi|_B$ and hence $S_{vN}[\rho_{AB}(t)] = 0$ which would violate (6.16). Thus, we can deduce that the conclusions in [Nakazato *et al.* 2003] for the case of selective measurements do not hold in the case of nonselective measurements as described by the double commutator master equation.

In fact, the H-theorem (6.16) implies that if by any chance the master equation (6.14) did result in any purification of the subsystem B then the entropy of A would necessarily increase. Nonetheless, the master equation (6.14) is not without some interesting properties. As mentioned before, independently of whether $\rho_A(0) = \text{Tr}_B\{\rho_{AB}(0)\}$ is such that $[M_A, \rho_A(0)] = 0$ or not, in the quantum Zeno limit the non-selective continuous monitoring of A will, for all practical purposes, freeze the dynamics of the subsystem A . However, depending on the interaction term in the Hamiltonian and on how fast the freezing settles in, this might result in the subsystem B behaving as if it were an isolated system with Hamiltonian dynamics.

To understand this last statement notice that, in general, the double commutator will result in the damping of the A -variables that do not commute with M_A (ultimately driving them to zero) but also in the stationarity of those that do commute. Depending on the interaction term in the Hamiltonian, this can be equivalent to the disappearance of the coupling terms between A and B , thus yielding the (near) equivalent of the closed dynamics for subsystem B . However, for this scenario to work (and be non-trivial), the monitoring needs to be effective enough (as controlled by the value of γ) so as the stationarity of the terms directly affected by the double

²The H-theorem in classical statistical mechanics refers to the agreement, in the mean, between the Boltzmann equation and the second law of thermodynamics. An interesting historical account of this subject can be found in [Ehrenfest 1959].

commutator is sufficiently well established before the damping effects propagate significantly to B (if the transient regime before stationarity is not short enough the state of B will be driven to the maximally mixed state, which is stationary even in the case of closed system dynamics). These concepts will be illustrated in the example presented in the next section.

6.4.3 An example

To illustrate the previous points let us consider the following example. Suppose the system of interest consists of two interacting two-level systems, A and B , whose Hamiltonian is:

$$H_{AB} = \frac{\omega_A}{2} (\sigma_z^A + 1) + \frac{\omega_B}{2} (\sigma_z^B + 1) + \mu (\sigma_+^A \sigma_-^B + \sigma_-^A \sigma_+^B), \quad (6.17)$$

where as usual $\sigma_k^{A(B)}$ ($k = x, y, z$) are the Pauli operators of system A (or B), and $\sigma_{\pm} = (\sigma_x \pm i\sigma_y)/2$.

This Hamiltonian corresponds to an example studied in the follow-up paper [Nakazato *et al.* 2004] and is capable of resulting in the aforementioned purification in the selective quantum Zeno limit. In the particular case studied, they consider an initial state of the composite system given by $\rho_{AB}(0) = |+\rangle_A \langle +| \otimes (|+\rangle_B \langle +| + |-\rangle_B \langle -|)/2$ and they fix the Hamiltonian parameters as $\omega_A = 5$, $\omega_B = 6$, all in units such that $\mu = 1$. After repeatedly confirming the state of A to be $|+\rangle$ the state of subsystem B is driven to a pure state with a success probability of $\frac{1}{2}$ (in the quantum Zeno limit).

Therefore, according to our previous discussions, the equivalent model in the case of continuous non-selective measurements would be

$$\frac{d}{dt}\rho_{AB} = -i[H_{AB}, \rho_{AB}] - \gamma [\sigma_z^A \otimes \mathbf{1}_B, [\sigma_z^A \otimes \mathbf{1}_B, \rho_{AB}]], \quad (6.18)$$

with H_{AB} given in (6.17).

Taking away the normalization condition, the master equation can be transformed into a set of fifteen differential equations for the quantities $\langle \sigma_{\alpha}^A \otimes \sigma_{\beta}^B \rangle_{\rho_{AB}(t)}$ ($\alpha, \beta = 0, x, y, z$; and $\sigma_0 = \mathbf{1}$). These equations are written in appendix D. Observe that not all the resulting equations are coupled, in fact the whole set can be decomposed into four subsets of coupled differential equations: one formed of 6 coupled equations, two with 4 coupled components, and the term $\langle \sigma_z^A \otimes \sigma_z^B \rangle$ is completely decoupled from the rest (and is a constant). Nonetheless, because of the complexity of the system (mainly due to the set of six coupled differential equations), we have not solved the problem analytically. Instead we have opted to integrate them numerically³ using the same Hamiltonian parameters as in the example cited above used in [Nakazato *et al.* 2004].

If we consider the same initial state as in [Nakazato *et al.* 2004], namely $\rho_{AB}(0) = |+\rangle_A \langle +| \otimes (|+\rangle_B \langle +| + |-\rangle_B \langle -|)/2$, in the Zeno limit (large γ) the state of subsystem A will be preserved (see figure 6.1). However, just as expected from the discussion in the previous section, the state of subsystem B is also conserved, and therefore there is no change in its purity. (We have not included a plot of the properties of B in this case because they simply result in a straight line similar to the one in figure 6.1 but centred at the origin).

³The numerical integrations were performed using the command NDSolve in Mathematica version 5.1

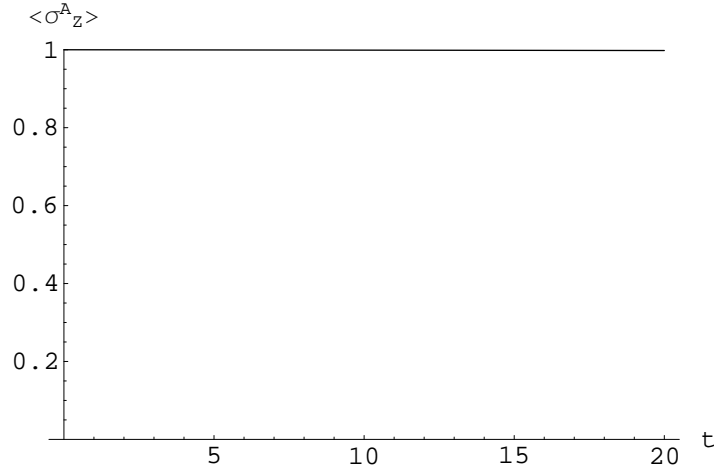


Figure 6.1: Plot of $\langle \sigma_z^A \rangle(t)$ obtained from the numerical integration of the master equation (6.18) for $\omega_A = 5$, $\omega_B = 6$, $\gamma = 5 \cdot 10^3$ in units such that $\mu = 1$, and the initial state $\rho_{AB}(0) = |+\rangle_A \langle +| \otimes (|+\rangle_B \langle +| + |-\rangle_B \langle -|)/2$.

Nonetheless, the model under consideration also serves to illustrate the “interesting” properties mentioned at the end of the previous section. For this, let us change the initial state to

$$\rho_{AB}(0) = |\rightarrow\rangle_A \langle \rightarrow| \otimes |\rightarrow\rangle_B \langle \rightarrow|,$$

where $|\rightarrow\rangle$ is the $+1$ eigenstate of σ_x .

Since $[\sigma_z^A, |\rightarrow\rangle_A \langle \rightarrow|] \neq 0$ the state of subsystem A , described $\rho_A = \text{Tr}_B \{\rho_{AB}\}$, will be driven to the maximally mixed state and its purity (as measured by $\text{Tr} \{\rho_A^2\}$) will decay to zero with a characteristic time-scale of $1/\gamma$. This is shown in figure 6.2. However, this particular example satisfies the conditions mentioned at the end of the last section, and in the Zeno limit (large γ) the dynamics of B will effectively correspond to those of an isolated system (see figure 6.3). This behaviour needs to be contrasted with what one obtains in the cases of ineffective monitoring (small γ), and of absolutely no monitoring ($\gamma = 0$, i.e. a closed AB system) shown in figures 6.4 and 6.5 respectively.

This previous phenomenon is easy to understand if we analyse the equations of motion (presented in appendix D) generated from the master equation. The continuous monitoring encoded in the double commutator term results in equations of the form

$$\frac{d}{dt} \langle \sigma_\alpha^A \otimes \sigma_\beta^B \rangle = -4\gamma \langle \sigma_\alpha^A \otimes \sigma_\beta^B \rangle + \dots$$

The components affected by this damping are $\langle \sigma_x^A \rangle$, $\langle \sigma_y^A \rangle$, $\langle \sigma_x^A \otimes \sigma_z^B \rangle$, $\langle \sigma_y^A \otimes \sigma_z^B \rangle$, $\langle \sigma_x^A \otimes \sigma_x^B \rangle$, $\langle \sigma_y^A \otimes \sigma_x^B \rangle$, $\langle \sigma_x^A \otimes \sigma_y^B \rangle$, and $\langle \sigma_y^A \otimes \sigma_y^B \rangle$. For sufficiently large values of γ all these components will quickly decay to zero (after a transient time period of the order of $1/\gamma$). Therefore, for times

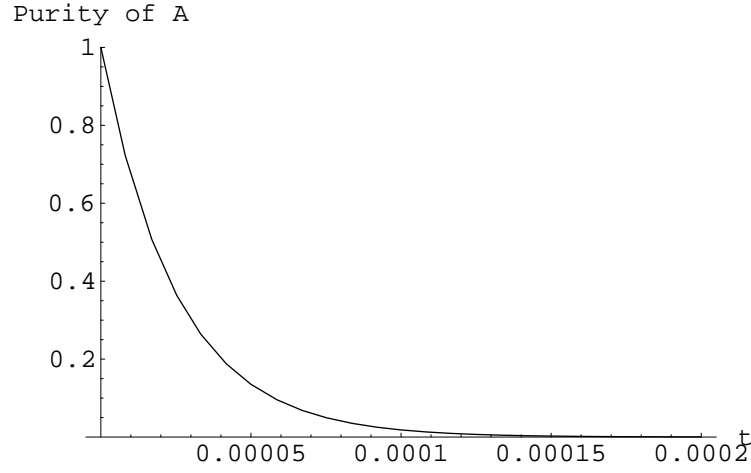


Figure 6.2: Purity of subsystem A ($\text{Tr} \{\rho_A^2(t)\}$) obtained from the numerical integration of the master equation (6.18) for $\omega_A = 5$, $\omega_B = 6$, $\gamma = 5 \cdot 10^3$ in units such that $\mu = 1$, and the initial state $\rho_{AB}(0) = |\rightarrow\rangle_A \langle \leftarrow| \otimes |\rightarrow\rangle_B \langle \leftarrow|$.

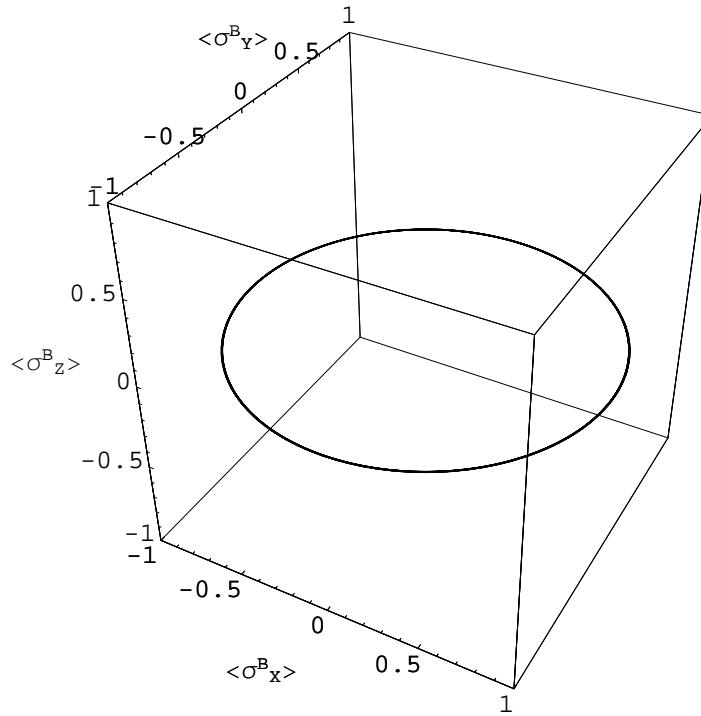
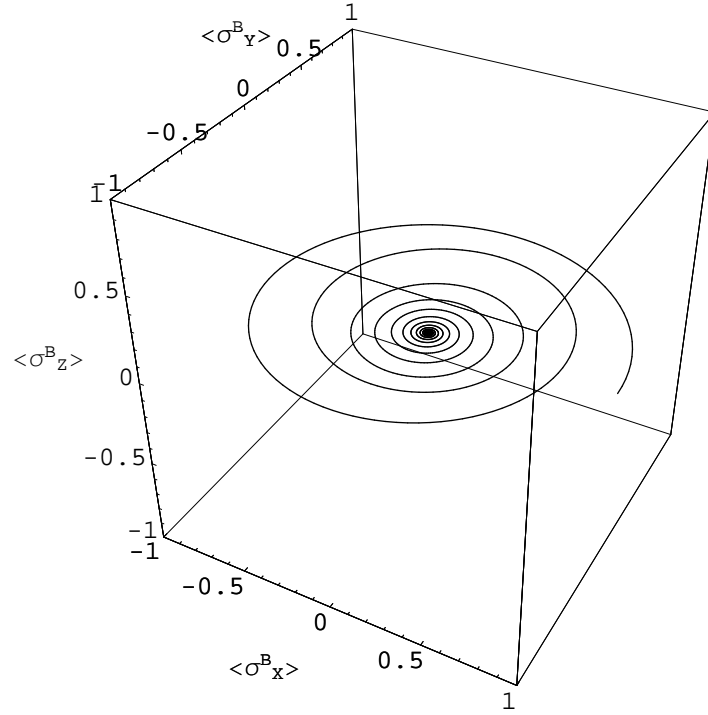


Figure 6.3: Parametric plot of the state of subsystem B obtained from the numerical integration of the master equation (6.18) for $\omega_A = 5$, $\omega_B = 6$, $\gamma = 5 \cdot 10^3$ in units such that $\mu = 1$, and the initial state $\rho_{AB}(0) = |\rightarrow\rangle_A \langle \leftarrow| \otimes |\rightarrow\rangle_B \langle \leftarrow|$ in the time region $t \in [0, 20]$.

Figure 6.4: Same as in figure 6.3 but with $\gamma = 2$.

$t > 1/\gamma$, the dynamics of the subsystem B will, for all intents and purposes, be given by:

$$\frac{d}{dt} \langle \sigma_x^B \rangle = -\omega_B \langle \sigma_y^B \rangle, \quad (6.19a)$$

$$\frac{d}{dt} \langle \sigma_y^B \rangle = \omega_B \langle \sigma_x^B \rangle, \quad (6.19b)$$

$$\frac{d}{dt} \langle \sigma_z^B \rangle = 0. \quad (6.19c)$$

This obviously corresponds to the equivalent of closed system dynamics dictated by the Hamiltonian $H_B = \frac{\omega_B}{2} (\sigma_z^B + 1)$. (The other equations that survive are those for $\langle \sigma_z^A \otimes \sigma_x^B \rangle$, $\langle \sigma_z^A \otimes \sigma_y^B \rangle$, $\langle \sigma_z^A \otimes \sigma_z^B \rangle$, and the Zeno term $\frac{d}{dt} \langle \sigma_z^A \rangle = 0$).

The effective initial condition to be used with the new set of equations (6.19) will depend on the time when the transient regime has passed and stationarity has settled in for the damped variables. The particular example shown above in figure 6.3 is such that the damping takes place sufficiently fast for the effective initial state of B to be almost a pure state. The apparent thickness of the orbit in figure 6.3 arises because of transient effects which entail an effective initial condition that is not exactly a pure state. If $\mu < \min\{\omega_A, \omega_B\}$ and we decrease the value of γ , the trajectory of the state of B will stabilize into an orbit with a smaller radius until the orbit will cease to exist when $\gamma \simeq \max\{\omega_A, \omega_B\}$ (in this case B is driven to the maximally mixed state $\frac{1}{2}\mathbf{1}$ before the stationary regime settles in). If the interaction coupling is such that $\mu > \max\{\omega_A, \omega_B\}$ then the damping will propagate faster to B and to have a stable orbit with

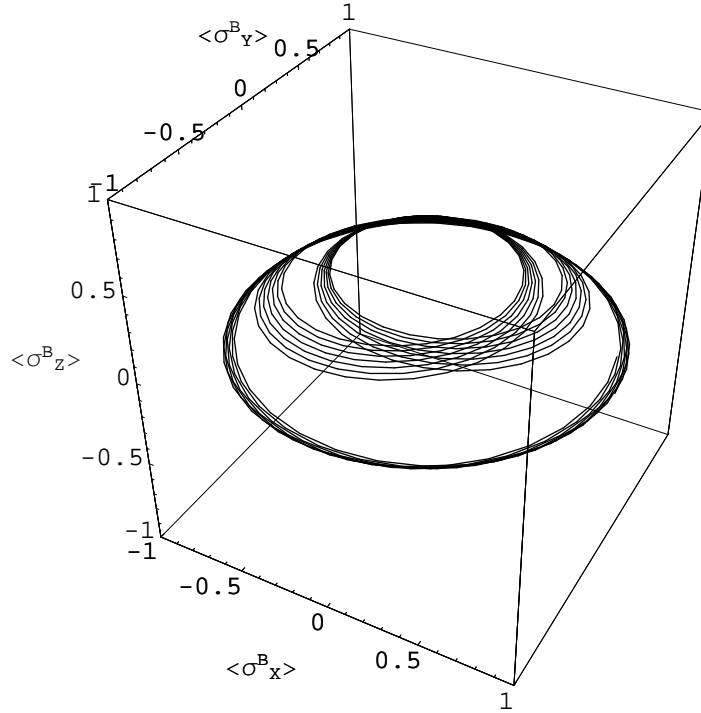


Figure 6.5: Same as in figure 6.3 but with $\gamma = 0$ (i.e. when the composite system AB is closed).

a non-zero radius we will need even larger values of γ (if not, the effective initial condition will be the maximally mixed state which would yield a unique fixed point for all future times).

To summarize, we have presented an example where the non-selective continuous monitoring, in the quantum Zeno limit, freezes the dynamics of a two-level system A interacting with another two-level system B . However, contrary to the case of selective projective measurements, the monitoring of A does not result in a purification of the state of B . In principle this should provide an experimentally verifiable condition to distinguish between the standard Copenhagen interpretation and other non-conventional interpretations/theories of quantum mechanics when they use a stochastic collapse model (see section 3.6) resulting in the master equation (6.9) as an alternative to projective measurements [GRW 1986] [Gisin & Percival 1992] [Pearle 1993] [Adler 2004]. Nevertheless, we must emphasize that this test would only serve to rule out some of the stochastic collapse models, but not all. This is because the stochastic Schrödinger equations are constructed *ad hoc*, and not all of them are equivalent to the double commutator master equation studied here. For example, in Percival’s quantum state diffusion interpretation, the test suggested here would only serve if for the description one chose a single Hermitian operator, $V = V^\dagger$, in equation (3.29).

Apart from these interpretational issues, we have also seen that the non-selective case is not without some interesting features. In particular we have shown that, for suitable system parameters, the freezing of A can result in B behaving as if it were isolated. It is our opinion that a similar technique could be used as an alternative to others, such as “decoherence-free subspaces”,

to protect quantum information in quantum computers (see for example [Lidar *et al.* 1998], and references therein). The scheme would involve embedding the system of interest, containing the relevant information, in a “cage” such that the system of interest only couples with the noise field through its interaction with the cage. A further study of such a scheme remains as future work.

Chapter 7

Critical Phenomena in Models of the Q-C Transition

In this chapter we will briefly explore the possibility of critical phenomena in the transition between the quantum and classical regimes. In the first section we present a series of examples that, for a suitable definition of quantumness, could be interpreted as corresponding to a critical Q-C transition. In the second section we extrapolate some concepts from the theory of phase transitions so as to suggest that they could be used in the description of the Q-C transition.

7.1 Some possible examples of criticality in the Q-C transition

Before delving into some examples that could be argued to lead to critical behaviour in the transition between quantum and classical regimes let us remind the reader that for a many-body system composed of N identical particles, and in the state ρ_T , the quantity

$$\langle i | \rho^{(1)} | j \rangle = \text{Tr} \{ \hat{\psi}_i \rho_T \hat{\psi}_j^\dagger \} = \langle \hat{\psi}_j^\dagger \hat{\psi}_i \rangle,$$

(where i, j represent single particles states) corresponds, up to a normalization constant of $1/N$, to the density matrix associated with just one of one of all the identical particles. Thus, $\rho^{(1)}$ is usually called the one-particle density matrix [Feynman 1972].

Bearing this concept in mind it is worthwhile noticing that for several systems the criteria used to distinguish a phase transition are very similar to the conditions used to characterize a pure quantum state introduced in section 1.3.

Our first example is the case of superfluids. [Penrose & Onsager 1956] proposed the criterion

$$\langle \hat{\psi}^\dagger(x) \hat{\psi}(y) \rangle \xrightarrow{|y-x| \rightarrow \infty} \langle \hat{\psi}^\dagger(x) \rangle \langle \hat{\psi}(y) \rangle,$$

to characterize the presence of off-diagonal long-range order (ODLRO) in the superfluid phase. Observe that this factorization of the single-particle density matrix is very similar to the one for pure states in (1.18).

Similarly, [Yang 62] showed that the existence of ODLRO in the superfluid phase is equivalent to $\langle \hat{\psi}^\dagger(x) \hat{\psi}(y) \rangle$ having an eigenvalue of order N . Thus, this is equivalent to the associated

density matrix $\frac{1}{N}\rho^{(1)}$ having a maximum eigenvalue of order one which is also one of the properties of pure states, see equation (1.17).

As is well known, the transition to the superfluid phase is a critical phenomenon occurring for temperatures below a critical value [Feynman 1972]. Thus, if we modified our criterion for quantumness to having a pure quantum state, this could provide an example of a critical C-Q transition. For future reference let us also point out that the temperature is also a property of the heat bath, i.e. the environment.

Another example is the laser. The coherence properties of the laser field are characterized by [Glauber 1963]:

$$\langle \hat{\psi}^\dagger(x, t) \hat{\psi}(y, t) \rangle = \langle \hat{\psi}^\dagger(x, t) \rangle \langle \hat{\psi}(y, t) \rangle.$$

This coincides exactly with the factorization property of pure states, equation (1.18). Similarly, the laser state is well known to occur only for pumping strengths above a critical threshold [Haken 1970]. This pumping strength is also a property of the environment. So, if we accepted this coherence as another example of quantum behaviour, we would have yet another example of critical behaviour.

The previous examples consist of many-body systems of interest where cooperative phenomena are involved. However we have already encountered an example of a single quantum system where the presence of quantum behaviour is arguably dependent on a critical parameter of the environment. Namely, in our simple example of section 6.4.1 of a two-level system obeying the dynamics dictated by a double commutator master equation, we saw that the presence of (damped) oscillations depends on the noise strength, characterized by γ , being below a critical value, viz. $\gamma < \omega$ (ω is the natural frequency of the system of interest). It would not be unreasonable to characterize the presence of quantum behaviour as coinciding with the presence of these oscillations, albeit damped.

In fact, there are several models of a two-level system interacting with a collection of bosons, where the presence of coherent motion (oscillations), though damped, depends on the coupling strength with the environment being below a critical value [Breuer & Petruccione 2002] (this critical value will obviously depend on the criterion of coherent motion being used, but the critical behaviour, together with the damping, is always present [Egger *et al.* 1997]).

Thus, if we took the presence of oscillatory motion as a condition of quantum behaviour, we have another example where quantumness will depend on an environment parameter satisfying a critical relation.

Even the simplistic example of a double-slit experiment can be argued to present aspects of criticality. Interference fringes will only be observed if the wavelength of the measured system is smaller than the slit separation. However, here we have two aspects to the origin of this criticality. One way this criticality arises is through the choices of the observer when setting up the experiment. The other, which is more similar to the ones presented above, arises because the environment affects the wavelength of the measured system by changing its momentum or it affects what would be the effective separation of the slits.

An interesting experimental example of this could be provided by the interferometry experiments on C_{70} fullerene molecules presented in [Hackermüller *et al.* 2004]. Figure 7.1 shows

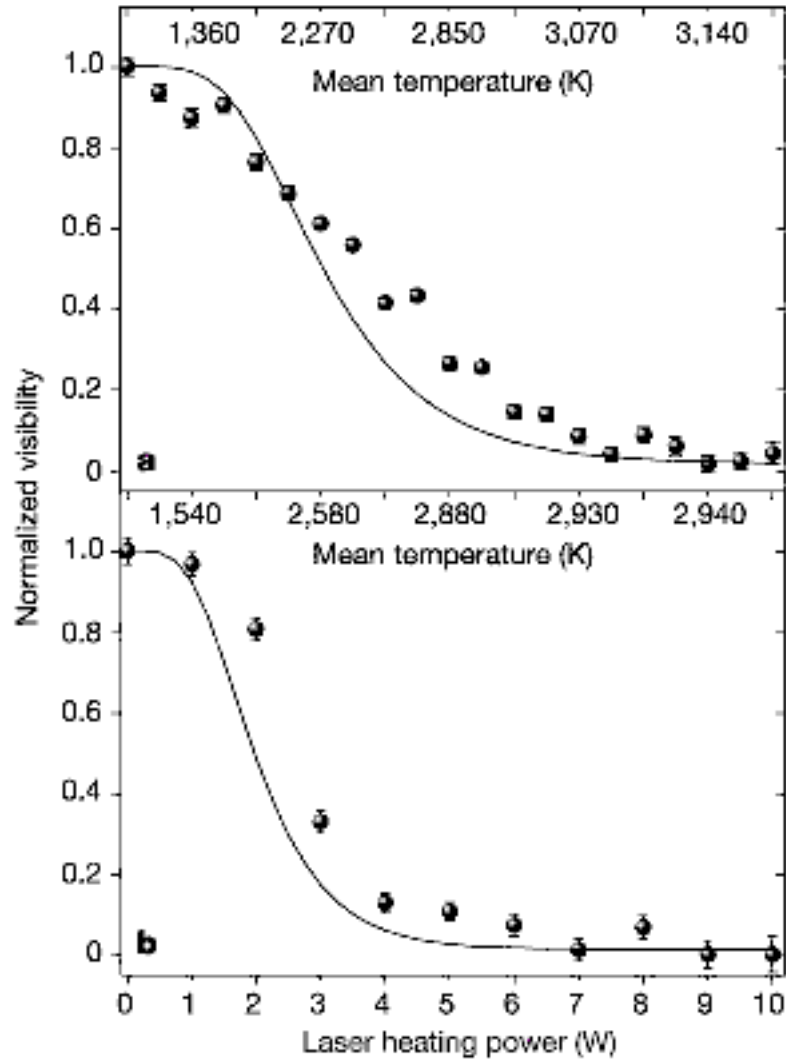


Figure 7.1: Figure taken from [Hackermüller *et al.* 2004] showing the normalized interference visibility of C_{70} fullerene molecules in a Talbot-Lau interferometer, for two different molecular beam mean velocities, as a function of laser heating power. The solid line corresponds to the theoretical prediction.

their results demonstrating how the normalized visibility (fringe contrast) depends on the heating power of the laser. The latter regulates the effective internal temperature of the fullerene molecules.

Apart from being a very interesting experiment showing that one can observe the wave properties of rather large molecules, it is our opinion that the normalized visibility curves show features similar to those one would expect from *finite-size* effects in a phase transition if we took the normalized visibility as the order parameter. Namely, we believe the figure could be loosely interpreted as the blurring of a critical transition at a temperature somewhere in the temperature range of 1300 K to 3000 K (because of dynamical effects the transition temperature would depend on the mean velocity of the molecular beam).

This finite-size behaviour is exactly what we would expect from this system, since the (main) environment affecting the center-of-mass variable being measured corresponds to the 204 vibrational modes of the molecule; definitely not a system in the thermodynamic limit necessary to observe critical behaviour [Huang 1987].

To better understand this, notice that the theoretical model used in [Hackermüller *et al.* 2004], which corresponds to the solid line in the curves, which essentially consists of decoherence arising from the recoil of the emission of thermal photons from the vibrational modes, states that the visibility V is given by

$$V = V_0 \exp \left\{ \int_0^{2L/v} dt \int d\lambda R(\lambda, t, Z_{204}(T)) \times g(d, \lambda, L, v, t) \right\}.$$

The exact form of all the terms is given in [Hackermüller *et al.* 2004], our interest here lies only in the fact that the visibility depends on the temperature only through the partition function of the 204 vibrational modes, denoted by $Z_{204}(T)$, and that $R(x, y, z)$ is an analytic function of its arguments. Thus, it is easy to see why we should expect finite-size effects in this system. If we wanted to observe critical behaviour, i.e. some sort of singularity in the visibility, as a function of temperature, this could only be achieved through the presence of singularities in the partition function $Z_{204}(T)$ (although, due to the dynamical effects -time of flight-, the exact location of the critical value will depend on the mean velocity of the molecular beam). However, as is well known, the partition function can only present singularities in the thermodynamic limit [Ruelle 1969], i.e. when the number of modes tends to infinity. Thus, this explains the presence of finite-size effects.

7.2 Commutativity and broken symmetries

Bearing in mind the examples presented in the previous section we believe it is natural to ask whether there are concepts from the theory of phase transitions that could be relevant in the study of the Q-C transition in the case of finite dimensional systems. We are particularly thinking of the concepts of broken symmetry and the order parameter [Anderson 1984].

In section 1.4 we already saw some of the features distinguishing a classical state space from a quantum one. In particular we saw that, because of the superposition principle and/or the non-commutativity of the observables, the quantum state space is not a simplex whilst the classical state space is a simplex. This, by itself, represents a considerable difference in the symmetry properties obeyed by the C and Q state spaces. As a simple illustration, figure 7.2 shows two



Figure 7.2: Example of two convex sets, one which is a simplex and another that is not.

convex sets, one that is a simplex and one that is not. The difference in symmetry is obvious. Thus, we would like to express this difference in a more rigorous language.

Since the main difference between the classical and quantum state spaces lies in the properties of its extreme points let us focus on the sets $\partial\tilde{C}$ and $\partial S(\mathfrak{A})$. Furthermore, as we have done in most of this thesis, let us define classicality with respect to the fine-grained partition $\{P_\mu\}_{\mu=1}^N$ of the Hilbert space, \mathfrak{H} , of the system of interest ($\dim\{\mathfrak{H}\} = N$). In this case the set of extreme classical points will coincide with the partition, i.e.

$$\partial\tilde{C}_{\{P_\mu\}} = \left\{ P_\mu \in \partial S(\mathfrak{A}) \mid P_\mu P_\nu = \delta_{\mu\nu} P_\mu, \sum_{\mu=1}^N P_\mu = \mathbf{1} \right\}.$$

The set $\partial S(\mathfrak{A})$ is simply composed of all the state vectors in the Hilbert space \mathfrak{H} , viz:

$$\partial S(\mathfrak{A}) = \{ \Psi \in S(\mathfrak{A}) \mid \Psi = |\psi\rangle\langle\psi|; |\psi\rangle \in \mathfrak{H} \}.$$

One of the key assumptions of Quantum Mechanics is the superposition principle, which states that the linear combination of state-vectors is itself a state vector [Dirac 58]. This translates to the fact that the unitary transformation of any pure state is again a state vector. That is, for *any* unitary operator U ($U \in \mathfrak{B}(\mathfrak{H})$, $U^\dagger U = \mathbf{1}$) we have that

$$\forall \Psi \in \partial S(\mathfrak{A}) \quad \exists \Psi' \in \partial S(\mathfrak{A}) \quad s.t. \quad U \Psi U^\dagger = \Psi'.$$

Hence, the set $\partial S(\mathfrak{A})$ obeys the symmetry that it is mapped into itself by *any* unitary transformation. Let us denote the set of all the unitary transformations by \tilde{U} .

However, notice that this symmetry no longer holds for the set of classical extreme states $\partial\tilde{C}_{\{P_\mu\}}$. In fact the set $\partial\tilde{C}_{\{P_\mu\}}$ will only be transformed into itself under the action of permutations amongst the labels of its elements. The group of permutations is only a small subset of the set of all the unitary transformations \tilde{U} .

Therefore we can qualitatively say that there is a *broken symmetry* involved when going from quantum to classical behaviour. The symmetry group of the set $\partial\tilde{C}_{\{P_\mu\}} \subset \partial S(\mathfrak{A})$ will necessarily be smaller than that of the set $\partial S(\mathfrak{A})$.

Now let us notice that in the theory of phase transitions the order parameter is in practice an object used to denote the restricted ensemble associated with the broken symmetry, contained

in the grand canonical ensemble [Josephson 1962] [Anderson 1984]. (Notice that, because of the broken symmetry, the restricted ensemble is contained but is not equal to the grand canonical ensemble which contains states respecting all the symmetries of the Hamiltonian).

Thus, an obvious choice for a possible order parameter could be the set $\partial\tilde{C}_{\{P_\mu\}}$ itself. The collection of projectors $\{P_\mu\}_{\mu=1}^N$ forming the partition will uniquely characterize the restricted set of states corresponding to classical behaviour.

To conclude, in analogy to the theory of phase transitions, we have been able to identify a “type” of broken symmetry and order parameter distinguishing the classical state space from the quantum one. However, there are some big differences. In the case of a “thermal” phase transition the symmetries refer to those transformations that leave the equilibrium state of the system invariant. In contrast, the symmetry we are talking about for the Q-C transition refers to the fact that *all* the pure states accessible to a quantum system lie on the same equivalence class, i.e. the symmetry refers to all of the state space and not to a particular one of the possible states that could be assigned to the system. As well, the arguments used above have explicitly made use of a finite-dimensional system. It is not clear we should expect a critical point in this case. In the last example of the previous section we have already put some arguments as to the blurring of a phase transition due to finite-size effects. Similarly, if we took a mathematically rigorous attitude, all the dynamical examples of decoherence we have encountered only result in a classical state asymptotically for $t \gg \tau_{dec}$.

Finally, it is important to mention that the question of a Q-C phase transition has been previously studied by other authors. Namely, [Aharonov 2000] has found that there is a phase transition from quantum to classical, in the context of quantum information, when Q behaviour is understood as the presence of entanglement. It remains as future work to see if the concepts introduced in this section could complement the description of the phase transition in [Aharonov 2000].

Chapter 8

Conclusions

We close this thesis by gathering the main results from the previous chapters. We highlight the areas where original contributions have been made and identify directions for future research.

The main philosophy used in this thesis has been to take for granted that there existed states that could be labelled as classical within the standard Quantum Theory, that is we accepted this theory to be generally valid. Under this assumption we defined a criterion for the classicality of states contained in the usual state space of non-relativistic Quantum Mechanics, and we chose to term all the other states as quantum (non-classical). Then, we aimed to develop an understanding of the transition between quantum (Q) and classical (C) behaviour, in *both* directions, mainly from a dynamical perspective. As well, whenever possible we have attempted to make reference to existing experimental results to justify our theoretical arguments.

In chapter 2 we studied some of the aspects related to detecting quantum behaviour. This work lead us to the novel realization that the limitations imposed by the Wigner-Araki-Yanase (WAY) theorem should also be taken into consideration for the case of weak measurements. This in turn drove us to study the possible implications of errors of the general form of those needed to by-pass the WAY theorem in the case of weak measurements coupled to post-selection. However, the model we used does not represent a solution to the WAY theorem when the conserved global variable is the total angular momentum. For further research on this topic, one could try to modify the example in [Ghirardi *et al.* 1981b], which does overcome the WAY theorem when the global variable is the total angular momentum, so as to include a larger spectrum for the probe and then see if in this case the conclusions of [Aharonov *et al.* 1988] still hold.

In chapter 2 we also pointed out some well known facts related to the contextuality of our definition of classicality, and we used an existing compatibility criterion to provide an original, and rigorous, argument towards the ambiguities of the Q-C question when two observers have previously agreed on the definition of classicality. In this case a possibly interesting line of research would be the analysis of the Q-C question when the observers have not agreed previously on the definition of classicality.

Chapter 3 was used to introduce some necessary tools for the description of the dynamics of open systems. Although no original results were included in this chapter, in section 3.5 we pointed out the unnecessary complexity of the work in [Stelmachovic & Buzek 2001] and gave several mathematical and physical arguments to justify the use of dynamical evolutions restricted to a proper subset of the state space.

In chapter 4 we used these tools to study dynamical transition from Q to C under the framework of decoherence theory. The main result in this chapter was the dependence of the general conclusions of decoherence theory on the choice of the initial state of the total system (system of interest plus environment). In particular we showed, in a specific model frequently used in the quantum computation literature to describe decoherence, that considering an initially correlated state can have dramatic consequences ranging from the existence of residual coherence to the production of pure quantum states. We left as future work the choice of a concrete physical example so as to fix the value of the constants determining the exact magnitude and location of the novel effects we found.

In chapter 5, entitled “Coherence Creating Process”, we inverted the question and focused on how to go from C to Q. Apart from introducing a simple criterion for a map to produce a Q-state, one of the main results of this chapter was the introduction of an ansatz for the structure of a linear map, defined for all states, producing a pure quantum state for all initial conditions. We also showed that this fixed point transformation is the only option for linear maps taking sufficient mixed states into pure ones, and that in the case of non-Markovian completely positive maps this can only be achieved if the environment is in a pure state of the same dimension as that of the system of interest. As well, we studied some of the mathematical properties of the inverse of a generalized depolarizing channel. Further research could be done to see if this map has any physical meaning or if it is just a mathematical curiosity.

Chapter 6 studied how one can obtain pure quantum states through measurements. The main contribution here was the analysis of the nonselective continuous measurement, in the quantum Zeno regime, of a subsystem coupled to another unmonitored subsystem. We showed that the conclusions obtained by [Nakazato *et al.* 2003], in the case of selective measurements, were no longer valid in the non-selective case. This lead us to propose that this difference between the two cases could serve as an experimental criterion to judge the validity of certain stochastic collapse theories. A more concrete study of this remains as work to be done in the future. As well, we showed that, for the correct combination of system parameters, this model could result in the unmonitored subsystem behaving as a quantum coherent closed system. A further line of research for this would be to exploit a similar technique for the protection of quantum information.

In chapter 7 we explored the possibility of interpreting the Q-C transition as a critical phenomenon for some suitable systems. Our contribution here was to identify what could broadly be called the equivalent of a broken symmetry and order parameter in the Q-C transition. The possible line of research stemming from this would be to see if these concepts can provide a guiding light to study the phase transition in [Aharonov 2000].

Appendix A

Operator sum expansions

Consider a system described by a *finite* dimensional Hilbert space \mathfrak{H} of dimension N . Then, on the space of the algebra of observables, defined to be the space of bounded observables over \mathfrak{H} , $\mathfrak{B}(\mathfrak{H})$, one can always construct a complete basis $\{B_\mu\}_{\mu=0}^{N^2-1}$ such that [Fano 1957] [Mahler & Weberruss 1998] [Schwinger 2001]:

$$\langle\langle B_\mu | B_\nu \rangle\rangle := \text{Tr} \left\{ B_\mu^\dagger B_\nu \right\} = N \delta_{\mu\nu}. \quad (\text{A.1})$$

Let us consider some examples. If $\{|i\rangle\}_{i=1}^N$ is a complete orthonormal basis for \mathfrak{H} , then we can build a set of basis operators as $B_{\mu=[ij]} = |i\rangle \langle j|$, we will call these types of bases “canonical bases”. Another option for a basis of $\mathfrak{B}(\mathfrak{H})$ could be to use the generators of the $\text{SU}(N)$ group. In this case the basis operators would be Hermitian and one of them would coincide with the identity element $\mathbf{1}_N$.

Thus, any operator can be written as¹

$$A = \frac{1}{N} B_\mu \langle\langle B_\mu | A \rangle\rangle, \quad (\text{A.2})$$

in particular the expansion of the density matrix reads:

$$\rho = \frac{1}{N} B_\mu \langle\langle B_\mu | \rho \rangle\rangle := \frac{\langle\langle B_\mu^\dagger \rangle\rangle}{N} \rho B_\mu. \quad (\text{A.3})$$

The Hilbert-Schmidt inner product of any two operators $A, B \in \mathfrak{B}(\mathfrak{H})$ can be written in terms of the components of the expansion (A.2) as:

$$\langle\langle A | C \rangle\rangle = \text{Tr} \left\{ A^\dagger C \right\} = \frac{1}{N} \overline{a_\mu} c_\mu,$$

where we have introduced the notation $a_\mu = \langle\langle B_\mu | A \rangle\rangle = \text{Tr} \left\{ B_\mu^\dagger A \right\}$.

In these operator expansions we are basically exploiting the vector space properties of $\mathfrak{B}(\mathfrak{H})$ (although it is possible to use these expansions to describe the multiplication of elements as well),

¹Throughout (except if stated otherwise) we will adopt the usual Einstein summation convention where repeated indices are summed over.

this has been emphasized by using a very similar notation to Dirac's for vectors of Hilbert spaces (actually, in the finite dimensional case being considered here, $\mathfrak{B}(\mathfrak{H})$ is itself a Hilbert space). Thus, it is only natural to also use this operator expansion formalism to describe the effect of endomorphisms over the vector space (we will call these superoperators). Thus, if we consider superoperators $\hat{\Lambda}$ such that $\hat{\Lambda} : \mathfrak{B}(\mathfrak{H}) \rightarrow \mathfrak{B}(\mathfrak{H})$ then due to the orthogonality of the basis we can schematically write the unit/identity superoperator as:

$$\hat{\mathbf{1}} = \frac{1}{N} |B_\mu\rangle\rangle\langle\langle B_\mu|,$$

and by inserting this superoperator wherever necessary the action of linear superoperators can be written as the multiplication of a vector by a matrix. Namely, if $C = \hat{\Lambda}A$ then we have that

$$c_\mu = \frac{1}{N} \Lambda_{\mu\nu} a_\nu,$$

where we have used the notation

$$\Lambda_{\mu\nu} = \langle\langle B_\mu | \hat{\Lambda} | B_\nu \rangle\rangle = \text{Tr} \left\{ B_\mu^\dagger \left(\hat{\Lambda} [B_\nu] \right) \right\}.$$

Furthermore, the composition of superoperators also obeys the usual matrix multiplication rules, e.g. if $\hat{\Lambda} = \hat{\Lambda}^{(1)} \hat{\Lambda}^{(2)}$ then

$$\Lambda_{\mu\nu} = \frac{1}{N} \Lambda_{\mu\alpha}^{(1)} \Lambda_{\alpha\nu}^{(2)}.$$

Just as in the “normal” case, we can change representations for the superoperators by the action of a unitary matrix. Namely, if $\Lambda_{\mu\nu}$ are the components of $\hat{\Lambda}$ in the basis $\left\{ B_\mu^{(1)} \right\}_{\mu=0}^{N^2-1}$, and Λ_{mn} are its components in the basis $\left\{ B_m^{(2)} \right\}_{m=0}^{N^2-1}$, then the components in both representations are related to each other as follows:

$$\Lambda_{\mu\nu} = u_{\mu m} \Lambda_{mn} \overline{u_{n\nu}},$$

where the scalars $u_{\mu m}$ form a unitary matrix with components given by:

$$u_{\mu m} = \langle\langle B_\mu^{(1)} | B_m^{(2)} \rangle\rangle.$$

For use in section 5.6 let us introduce some of these matrices. For example to go from the canonical basis formed by the eigenvectors of the Pauli operator σ_z , $\{|+\rangle\langle+|, |-\rangle\langle-|, |+\rangle\langle-|, |-\rangle\langle+|\}$, to the one formed by the eigenvectors of σ_x , $\{|\rightarrow\rangle\langle\rightarrow|, |\leftarrow\rangle\langle\leftarrow|, |\rightarrow\rangle\langle\leftarrow|, |\leftarrow\rangle\langle\rightarrow|\}$ (with $\sigma_x |\rightarrow\rangle = +|\rightarrow\rangle$ and $\sigma_x |\leftarrow\rangle = -|\leftarrow\rangle$), the unitary matrix is given by

$$\hat{U}_{X-Z} = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \end{pmatrix}. \quad (\text{A.4})$$

Similarly, to go from the basis formed by the eigenvectors of σ_z to the one formed by the generators of $\text{SU}(2)$, $\{\frac{1}{\sqrt{2}}, \frac{\sigma_x}{\sqrt{2}}, \frac{\sigma_y}{\sqrt{2}}, \frac{\sigma_z}{\sqrt{2}}\}$, the matrix reads:

$$\hat{U}_{SU-Z} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & i & -i \\ 1 & -1 & 0 & 0 \end{pmatrix}. \quad (\text{A.5})$$

Appendix B

Distances from $\frac{1}{n}$

First let us calculate the distance, as defined in equation (5.42), from $\frac{1}{n}$ to an arbitrary pure state $\Psi (=|\psi\rangle\langle\psi|)$. This is easily done if we use an orthonormal basis (for the Hilbert space) that contains $|\psi\rangle$ (which is always possible), then it is trivial to diagonalize the operator $(\Psi - \frac{1}{n})$ which yields:

$$\begin{aligned} d\left(\Psi, \frac{1}{n}\right) &= \text{Tr} \left\{ \left| \begin{pmatrix} 1 - \frac{1}{n} & & 0 \\ & -\frac{1}{n} & \\ & & \ddots \\ 0 & & & -\frac{1}{n} \end{pmatrix} \right| \right\} \\ &= \left(1 - \frac{1}{n}\right) + \frac{1}{n}(n-1) \\ &= 2\left(1 - \frac{1}{n}\right). \end{aligned} \tag{B.1}$$

(We have exploited the fact that the operator $\mathbf{1}$ is diagonal in any basis).

Now consider an arbitrary *mixed* state $\rho \in S(\mathfrak{A})$ (that is not a maximally mixed state $\frac{1}{n}$). The state can always be decomposed as $\rho = \sum_{i=1}^n \lambda_i |\lambda_i\rangle\langle\lambda_i|$, with $\langle\lambda_i|\lambda_j\rangle = \delta_{ij}$, and its eigenvalues satisfy $\sum_{i=1}^n \lambda_i = 1$, with $\lambda_i \geq 0$ (we will include in the spectrum all the zero eigenvalues, if any, and we will also include the null space in the decomposition). Let us split the spectrum of ρ into two sets defined as:

$$\begin{aligned} \tilde{L}_{\geq} &: = \{\lambda_i | \lambda_i \geq 1/n\}, \\ \tilde{L}_{<} &: = \{\lambda_j | \lambda_j < 1/n\}. \end{aligned}$$

For convenience we will use the notation:

$$\begin{aligned} n_{\geq} &: = \text{card} \left\{ \tilde{L}_{\geq} \right\}, \\ n_{<} &: = \text{card} \left\{ \tilde{L}_{<} \right\}. \end{aligned}$$

Since, by assumption, ρ is mixed and is not equal to the maximally mixed state, we have that $n_{\geq} \geq 1$, and $n_{<} \geq 1$. Also, because of the inclusion of the zero eigenvalues, we have the relation:

$$n_{\geq} + n_{<} = n. \tag{B.2}$$

Then we have that:

$$\begin{aligned} d\left(\rho, \frac{\mathbf{1}}{n}\right) &= \sum_{\lambda_i \in \tilde{L}_{\geq}} \left\{ \lambda_i - \frac{1}{n} \right\} + \sum_{\lambda_j \in \tilde{L}_{<}} \left\{ \frac{1}{n} - \lambda_j \right\} \\ &= \frac{n_{<} - n_{\geq}}{n} + \sum_{\lambda_i \in \tilde{L}_{\geq}} \lambda_i - \sum_{\lambda_j \in \tilde{L}_{<}} \lambda_j, \end{aligned}$$

which together with (B.1), and some simple algebra exploiting the normalization $\sum_{i=1}^n \lambda_i = 1$ and the relation (B.2) gives:

$$d\left(\psi, \frac{\mathbf{1}}{n}\right) - d\left(\rho, \frac{\mathbf{1}}{n}\right) = 2 \left(\frac{n_{\geq} - 1}{n} + 2 \sum_{\lambda_i \in \tilde{L}_{\geq}} \lambda_i \right).$$

But since $n_{\geq} \geq 1$, and $\lambda_i > 0$ for every i , we have that the rhs is strictly positive. Thus we have proven that a strictly mixed state satisfies the relation

$$d\left(\rho, \frac{\mathbf{1}}{n}\right) < d\left(\Psi, \frac{\mathbf{1}}{n}\right). \quad (\text{B.3})$$

This should answer any doubts the reader might of had as to the reason behind calling the pure states extreme states (at least for the finite dimensional case).

Appendix C

Derivation of the non-selective measurement master equation

To derive the master equation used in section 6.4 we follow closely the presentation in [Braginsky & Khalili 1992]. We will consider a system of interest, S , that is monitored by an “environment,” E , formed by N identical non-interacting quantum probes. As well we will suppose that the probes have a vanishing Hamiltonian (this simply means that the state of the probe is conserved before and after the interaction with S) and that they are initially prepared independently of each other, i.e.

$$\rho_E(0) = \bigotimes_{j=1}^N \rho_{pointer_j} \quad \text{with} \quad \rho_{pointer_j} = \rho_{ref} \quad \forall j, \quad (\text{C.1})$$

and

$$\rho_{S+E}(0) = \rho_S(0) \otimes \rho_E(0). \quad (\text{C.2})$$

Under these assumptions the Hamiltonian describing the total system, $S + E$, will be of the form¹

$$H_{SE} = H_S - \sum_{j=1}^N \lambda g_j(t) M q_j, \quad (\text{C.3})$$

where H_S is the Hamiltonian of S when it is a closed system, λ is a coupling constant, M is the observable of S that will be monitored and q_j is a pointer variable. The scalar function $g_j(t)$ has compact support over the interval

$$(j-1)\theta \leq t \leq j\theta, \quad (\text{C.4})$$

and is normalized such that $\int dt g_j(t) = 1$.

If θ is assumed to be arbitrarily small, the time evolution of the whole system during the

¹Actually, if we were more rigorous, the second term of \hat{H}_{SE} should be written as $\sum_{j=1}^N \lambda g_j(t) \hat{M} \otimes \left(\bigotimes_{k=1}^{j-1} \hat{1} \right) \otimes \hat{q}_j \otimes \left(\bigotimes_{l=j+1}^N \hat{1} \right)$

time interval (C.4), corresponding to the interaction of the j -th probe with S , can be written as:

$$\begin{aligned} U_j &= \exp \left\{ -\frac{i}{\hbar} (H_s - \lambda M q_j) \theta \right\} \\ &\simeq \mathbf{1} - \frac{i\theta}{\hbar} (H_s - \lambda M q_j) - \frac{\theta^2}{2\hbar^2} (H_s - \lambda M q_j)^2 + \dots \end{aligned} \quad (\text{C.5})$$

Let us denote the state of S at time $(j-1)\theta$ by ρ_j , i.e. $\rho_j \equiv \text{Tr}_E \{ \rho_{SE}((j-1)\theta) \}$. Then, if no observer measures (“collapses”) the state of the pointer, the system at the end of the j -th interaction will have evolved to the state

$$\rho_{j+1} = \text{Tr}_E \left\{ U_j \rho_j U_j^\dagger \right\}. \quad (\text{C.6})$$

By inserting into this the approximate expression for U_j given in (C.5) and keeping terms up to second order in θ we obtain

$$\begin{aligned} \rho_{j+1} &= \rho_j - \frac{i\theta}{\hbar} [H_s - \lambda M \langle q_j \rangle, \rho_j] - \frac{\theta^2}{2\hbar^2} [H_s, [H_s, \rho_j]] - \frac{\lambda^2 \theta^2}{2\hbar^2} \langle q_j^2 \rangle [M, [M, \rho_j]] \\ &\quad + \frac{\lambda \theta^2}{2\hbar^2} \langle q_j \rangle ([H_s, [M, \rho_j]] + [M, [H_s, \rho_j]]), \end{aligned} \quad (\text{C.7})$$

where the averages $\langle q_j \rangle$ and $\langle q_j^2 \rangle$ are taken over the reference state of the pointer ρ_{ref} .

Now let us make the following assumptions:

1. It is physically valid to take the limit $\theta \rightarrow 0$. (This assumption can be well justified for certain physical systems since femtosecond [Rabitz *et al.* 2000], and even attosecond [Baltusca *et al.* 2003], laser pulses are now widely available for the control of systems with spontaneous emission times of nanoseconds)
2. The initial state of the pointers, the reference state, has been set to “zero”, i.e.

$$\langle q_j \rangle = 0 \quad (\text{C.8})$$

3. Finally, we shall also assume that in the limit $\theta \rightarrow 0$ the quantity

$$\sigma_q^2 \equiv \theta \lambda^2 \langle q_j^2 \rangle \quad (\text{C.9})$$

remains constant and different from zero. (This will make the probe’s fluctuational back-action remain finite in the continuum limit. As well it can be shown that, the more precise the monitoring is, the larger σ_q will be [Braginsky & Khalili 1992]. The physical validity of this assumption is more difficult to justify since it is tantamount to the probes being delta correlated which, if we were rigorous, would require an infinite amount of energy. However, in practice, the validity of delta function correlations is also a time scale problem that can be justified if the correlation time is much shorter than any other characteristic time).

From these assumptions, and equation (C.7), it follows that

$$\lim_{\theta \rightarrow 0} \frac{\rho_{j+1} - \rho_j}{\theta} = -\frac{i}{\hbar} [H_s, \rho_j] - \frac{\sigma_q^2}{2\hbar^2} [M, [M, \rho_j]]. \quad (\text{C.10})$$

By taking the continuum limit we obtain the master equation for the state of S under continuous monitoring, viz:

$$\frac{d}{dt}\rho(t) = -\frac{i}{\hbar} [H_s, \rho(t)] - \frac{\sigma_q^2}{2\hbar^2} [M, [M, \rho(t)]] . \quad (\text{C.11})$$

Appendix D

Equations of motion for double commutator master equation

For the convenience of the reader we include here the equations of motion resulting from the master equation (6.14) in section 6.4.3. In the whole set of equations there are two constant terms, viz:

$$\begin{aligned}\frac{d}{dt}\langle \mathbf{1}_{AB} \rangle &= 0, \\ \frac{d}{dt}\langle \sigma_z^A \otimes \sigma_z^B \rangle &= 0.\end{aligned}$$

The first one corresponds to the conservation of the trace of the state.

The largest set of coupled differential equations corresponds to:

$$\begin{aligned}\frac{d}{dt}\langle \sigma_z^B \rangle &= \mu \langle \sigma_x^A \otimes \sigma_y^B \rangle - \mu \langle \sigma_y^A \otimes \sigma_x^B \rangle, \\ \frac{d}{dt}\langle \sigma_x^A \otimes \sigma_x^B \rangle &= -4\gamma \langle \sigma_x^A \otimes \sigma_x^B \rangle - \omega_B \langle \sigma_x^A \otimes \sigma_y^B \rangle - \omega_A \langle \sigma_y^A \otimes \sigma_x^B \rangle, \\ \frac{d}{dt}\langle \sigma_x^A \otimes \sigma_y^B \rangle &= -4\gamma \langle \sigma_x^A \otimes \sigma_y^B \rangle - \mu \langle \sigma_z^B \rangle + \omega_B \langle \sigma_x^A \otimes \sigma_x^B \rangle - \omega_A \langle \sigma_y^A \otimes \sigma_y^B \rangle + \mu \langle \sigma_z^A \rangle, \\ \frac{d}{dt}\langle \sigma_y^A \otimes \sigma_x^B \rangle &= -4\gamma \langle \sigma_y^A \otimes \sigma_x^B \rangle + \mu \langle \sigma_z^B \rangle + \omega_A \langle \sigma_x^A \otimes \sigma_x^B \rangle - \omega_B \langle \sigma_y^A \otimes \sigma_y^B \rangle - \mu \langle \sigma_z^A \rangle, \\ \frac{d}{dt}\langle \sigma_y^A \otimes \sigma_y^B \rangle &= -4\gamma \langle \sigma_y^A \otimes \sigma_y^B \rangle + \omega_A \langle \sigma_x^A \otimes \sigma_y^B \rangle + \omega_B \langle \sigma_y^A \otimes \sigma_x^B \rangle, \\ \frac{d}{dt}\langle \sigma_z^A \rangle &= -\mu \langle \sigma_x^A \otimes \sigma_y^B \rangle + \mu \langle \sigma_y^A \otimes \sigma_x^B \rangle.\end{aligned}$$

The rest of the equations result in the following two sets of coupled equations:

$$\begin{aligned}\frac{d}{dt}\langle \sigma_x^B \rangle &= -\omega_B \langle \sigma_y^B \rangle + \mu \langle \sigma_y^A \otimes \sigma_z^B \rangle, \\ \frac{d}{dt}\langle \sigma_y^B \rangle &= \omega_B \langle \sigma_x^B \rangle - \mu \langle \sigma_x^A \otimes \sigma_z^B \rangle, \\ \frac{d}{dt}\langle \sigma_x^A \otimes \sigma_z^B \rangle &= -4\gamma \langle \sigma_x^A \otimes \sigma_z^B \rangle + \mu \langle \sigma_y^B \rangle - \omega_A \langle \sigma_y^A \otimes \sigma_z^B \rangle, \\ \frac{d}{dt}\langle \sigma_y^A \otimes \sigma_z^B \rangle &= -4\gamma \langle \sigma_y^A \otimes \sigma_z^B \rangle - \mu \langle \sigma_x^B \rangle + \omega_A \langle \sigma_x^A \otimes \sigma_z^B \rangle,\end{aligned}$$

and

$$\begin{aligned}
\frac{d}{dt} \langle \sigma_x^A \rangle &= -4\gamma \langle \sigma_x^A \rangle - \omega_A \langle \sigma_y^A \rangle + \mu \langle \sigma_z^A \otimes \sigma_y^B \rangle, \\
\frac{d}{dt} \langle \sigma_y^A \rangle &= -4\gamma \langle \sigma_y^A \rangle + \omega_A \langle \sigma_x^A \rangle - \mu \langle \sigma_z^A \otimes \sigma_x^B \rangle, \\
\frac{d}{dt} \langle \sigma_z^A \otimes \sigma_x^B \rangle &= \mu \langle \sigma_y^A \rangle - \omega_B \langle \sigma_z^A \otimes \sigma_y^B \rangle, \\
\frac{d}{dt} \langle \sigma_z^A \otimes \sigma_y^B \rangle &= -\mu \langle \sigma_x^A \rangle + \omega_B \langle \sigma_z^A \otimes \sigma_x^B \rangle.
\end{aligned}$$

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